Advances in Cylindrical Algebraic Decomposition

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Summary

Since their conception by Collins in 1975, Cylindrical Algebraic Decompositions (CADs) have been used to analyse the real algebraic geometry of systems of polynomials. Applications for CAD technology range from quantifier elimination to robot motion planning. Although of great use in practice, the CAD algorithm was shown to have doubly exponential complexity with respect to the number of variables for the problem, which limits its use for large examples.

Due to the high complexity of CAD, much work has been done to improve its performance. In this thesis new advances will be discussed that improve the practical efficiency of CAD for a variety of problems, with a new complexity result for one set of algorithms.

A new invariance condition, truth table invariance (TTICAD), and two algorithms to construct TTICADs are given and shown to be highly efficient. The idea of restricting the output of CADs, allowing for greater efficiency, is formalised as sub-decompositions and two particular ideas are investigated in depth. Efficient selection of various formulation choices for a CAD problem are discussed, with a collection of heuristics investigated and machine learning applied to assist in choosing an optimal heuristic. The mathematical expression of a problem is shown to be of great importance, with preconditioning and reformulation investigated.

Finally, these advances are collected together in a general framework for applying CAD in an efficient manner to a given problem. It is shown that their combination is not cumulative and care must be taken. To this end, a prototype software CADassistant is described to help users take advantage of the advances without knowledge of the underlying theory.

The effects of the various advances are demonstrated through a guiding example originally considered by Solotareff, which describes the approximation of a cubic polynomial by a linear function. Naïvely applying CAD to the problem takes 916.1 seconds of construction (from which a solution can easily be derived), which is reduced to 20.1 seconds by combining various advances from this thesis.

Acknowledgements

I have been fortunate to have been surrounded and supported by some brilliant people whilst completing my doctoral research. Without those listed below, this thesis would not have been possible.

First, I would like to thank my supervisors, Prof. James H. Davenport and Dr Russell J. Bradford. I am forever grateful for their guidance and support during my studies and the opportunities they have given me. I consider myself very fortunate to have been their student and have gained much more than just academic knowledge under their supervision.

I would also like to thank Dr Matthew England and other collaborators (particularly Prof. McCallum, Prof. Moreno Maza, Prof. Chen, Miss Huang). Not only have I been able to complete interesting research with them, but also had an enjoyable time doing so.

Whilst studying for my Masters, I was inspired by Dr Doron Zeilberger to stop thinking of mathematics and computer science as separate subjects and instead look more deeply at their connection. Further, I am thankful to Dr Z. for the initial suggestion of applying Bath to work on computer algebra. I also wish to thank my tutors at Wadham College (Prof. Woodhouse, Dr Marshall, Dr Hodge) and teachers at Coquet High School (particularly Mr. Singh and Mrs. Adams) for nurturing my mathematical interest and encouraging me to pursue further study.

I have been lucky to have been surrounded by supportive and special friends. They have helped me through tough times and celebrated with me through happy times. Thanks to them, I've come through the last three years with a smile on my face.

Finally, I would not be where I am today without the endless support of my family: Mum, Dad, and James. They are a constant inspiration and I love them dearly. Thank you for everything over the last twenty-seven years, I owe it all to you.

D. J. W.

Table of Contents

List of Algorithms

List of Figures

List of Tables

Chapter 1

Introduction

We introduce the subject of this thesis, cylindrical algebraic decomposition (CAD). We illustrate the need for improvements in CAD and discuss how this thesis aims to meet those aims. After summarising the contributions of this thesis, we also identify a guiding example that will be considered throughout this thesis.

1.1 Motivation

Cylindrical Algebraic Decompositions (CADs) are mathematical structures that were introduced by Collins [Col75] as an algorithmic way to analyse the real algebraic geometry of a system of polynomials. A CAD decomposes real space into cells such that the input polynomials are invariant with respect to their sign on each cell. The standard method of constructing a CAD of $\mathbb{R}^n$ involves projecting the polynomials down to $\mathbb{R}^{n-1}, \ldots, \mathbb{R}^1$, before lifting, a variable at a time, back up to $\mathbb{R}^n$.

CAD construction can be used as a sub-procedure for a variety of applications, including Quantifier Elimination (QE) and verification of algebraic identities. Specialised algorithms exist for particular types of problems, but CAD remains one of the most useful general algorithms in this area.

The main issue with CAD is its inherent complexity. A CAD constructed with respect to a set of polynomials can end up containing a large number of cells: doubly exponential in the number of variables involved. Whilst this complexity limits the use of CAD for problems involving many variables, there is much room within the double exponential for improvements in efficiency.

The aim of this body work is to improve the efficiency of CAD within all areas of the algorithm: preconditioning and expression of the input, simplification of the projection,

restriction of the output during lifting, and the interaction between these advances.

1.2 Contribution of this Thesis

This thesis aims to present a variety of results that enable the construction of cylindrical algebraic decompositions (CADs) as efficiently as possible. This includes producing smaller and simpler CADs for existing problems as well as constructing CADs for problems that were previously infeasible.

A thorough survey of the literature around CAD will be given in Chapter 2 before the various advances in the theory of cylindrical algebraic decomposition are discussed. The work will be grouped in topics and presented in an approximately chronological order. The ideas will then be gathered in Chapter 7 to discuss their place within the overall framework and interactions.

We summarise the main topics and results:

- In Chapter 3 a new invariance condition for CAD is given. Mathematically verified algorithms are given to construct such CADs with two methods of CAD construction available, and thorough experimentation of all implementations is carried out.
- In Chapter 4 the idea of restricting the output of a CAD algorithm whilst retaining all important cells is formalised and discussed. Two key ideas, and their composition, are introduced and complexity results and experimental data are given.
- In Chapter 5 various decisions that are required to construct a CAD are investigated, with associated heuristics. The application of machine learning to one of these choices is investigated and the work in Chapter 4 is used in a new heuristic.
- In Chapter 6 the importance of finding an optimal mathematical description of a problem for CAD is shown. Preconditioning input by Gröbner bases is investigated and a classic CAD problem that was previously infeasible is reformulated to become possible. A general strategy for describing a problem mathematically is given.
- In Chapter 7 the interaction of all this work is discussed. A collection of examples proves that this can be non-trivial (with advances interfering with each other). A hierarchy of the advances is given along with a proof-of-concept tool, CADassistant, to assist in the decision-making process.
- In Chapter 8 various ideas for extending the work of this thesis are described, before a short recapitulation of the key results.

1.2.1 Stages of Solving a Problem With CAD

We put this work in context by briefly describing the general approach to solving a problem with CAD.

There are multiple stages to solving a problem with CAD, and decisions at all points can impact the feasibility of a problem. Informally, the decisions to be made are:

1. **Describing the problem mathematically** (discussed in Chapter 6);
2. **Formulating the problem for CAD**, including:
   (a) **Selecting a CAD algorithm/Selecting an invariance condition** (a new algorithm and invariance condition are discussed in Chapter 3);
   (b) **Choosing a variable ordering** (discussed in Chapter 5);
   (c) **Preconditioning input** (discussed in Chapter 6);
   (d) **Selecting various parameters** (discussed in Chapter 5);
3. **Restricting the output appropriately** (discussed in Chapter 4);
4. **Postprocessing the output CAD** (briefly discussed in Appendix A).

This process is not necessarily sequential (for example, preconditioning input depends on variable ordering) and this interaction is discussed in Chapter 7, which also presents a planning assistant to help navigate this complexity.

1.2.2 Author's Contribution

Much of the theoretical work in this thesis is collaborative, and through the publication process[1] nearly all topics have been developed collaboratively. Before each chapter and major section of work, the contribution of the author has been described. To summarise this contribution, most of the work in Chapter 4 (including its extension to the work of Section 5.4) and Chapter 6 was almost solely conducted by the author (with supervision from Prof. Davenport and Dr Bradford). The author contributed to the theoretical discussion and experimentation of the work in Chapter 3 and Chapter 5 at varying degrees in different sections of the work. The work in Chapter 7 is mainly unpublished and by the author.

[1] A full list of publications of the work in this thesis is given in Appendix E.

1.3 Guiding Example: Solotareff

Throughout this thesis, we will consider a guiding CAD example to demonstrate the key concepts. Solotareff first posed a question regarding polynomial approximations in 1933 and it was heavily discussed in [Ach56]. The general Solotareff problem is stated as the following.

Problem 1.1 (The Solotareff Problem)**.**
Find the best approximation, with respect to the uniform norm[2] on $[-1, 1]$, of a polynomial of degree n by a polynomial of degree $n - 2$ or less.

The Solotareff problem is clearly equivalent to approximating the binomial $x^n + rx^{n-1}$.

We will pay particular interest to the case where $n = 3$ and $r = -1$: finding the best approximation to the cubic polynomial $x^3 - x^2$ by a linear function $ax + b$.

This case was discussed in [BH91] and we will consider various ways the problem can be tackled by CAD throughout the thesis. Naïvely constructing a CAD by Collins' algorithm to solve this problem may result in up to $161,317$ cells in over 15 minutes, but this can be reduced to $1,603$ cells in 20 seconds using a new variant on that algorithm (based on various advances from this thesis), or as low as 42 and 29 cells using alternative CAD algorithms combined with advances from this thesis. These results are summarised and contrasted in Section 8.2.

1.4 Experimentation

Experiments in this thesis, unless stated otherwise, were completed on a Linux desktop (3.1GHz Intel processor, 8.0Gb total memory) with Maple 16 (command line interface), development Maple (command line interface), Mathematica 9 (graphical interface) and Qepcad-B 1.69. All graphs and figures were generated using either Maple 16-18 (graphical interface) or Qepcad-B 1.69.

The work in this thesis is necessarily heavily experimental. Clearly, the results of a finite set of examples cannot compare to a mathematical proof of the benefit (which is given wherever possible). However, for each piece of work all attempts have been made to give a diverse collection of examples to show the behaviour of a particular algorithm or technique. When possible, examples are sourced from the literature or applications of CAD, but this is not always feasible due to the work in this thesis expanding the scope

[2]The **uniform norm** on a set S, $\|f\|_{\infty,S}$, is defined to be $\sup\{|f(x)| \mid x \in S\}$.

of CAD. Finally, for any work that is not universally beneficial, examples highlighting the potential detrimental effect have been given to show the limitations of the theory.

1.5 Collaborators

As described earlier, the majority of the work in this thesis was completed in collaboration with other researchers. Every effort has been made to clarify which contributions were entirely from the author, and the author's role in each piece of research is hopefully clear.

The main collaborators are the University of Bath "Real Geometry and Connectedness via Triangular Description" research group, which consists of Prof. James H. Davenport, Dr Russell J. Bradford, Dr Matthew England, and the author. A seminar hosted by the research group (where many of the ideas in this thesis were discussed) included contributions from Prof. Gregory Sankaran, Acyr Locatelli, and Prof. Nicolai Vorobjov. External collaborators include Prof. Scott McCallum (Macquarie University, Australia), Prof. Marc Moreno Maza (Western University, Canada), Dr Changbo Chen (CIGIT, Chinese Academy of Sciences, China) and the automated theorem proving team at Cambridge University (Prof. Lawrence C. Paulson, Zongyan Huang and Dr James Bridge).

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Chapter 2

Background Material

Cylindrical Algebraic Decomposition (CAD) was introduced in 1975 by Collins [Col75] and has seen much research since. It has developed into a key tool to study real algebraic geometry and there now exists many variants of the original algorithm.

This chapter begins by recalling key concepts in computer algebra, which also serves to fix notation for use throughout this thesis. The original algorithm is described along with an analysis of its complexity. This is accompanied by a discussion of key improvements to CAD theory and applications of CAD. Finally, a small survey of alternatives to CAD is given, with their merits and demerits, along with a discussion of how CAD interacts with formalisation of mathematics.

2.1 Notation and Background Computer Algebra

We will standardise notation used throughout this thesis, along with providing some important background in computer algebra. Further background can be found in any good computer algebra textbook, such as [VZGG13].

2.1.1 Fields and Multivariate Polynomials

Let $\mathbb{N}$ denote the set of natural numbers (including 0), $\mathbb{Z}$ the ring of integers, $\mathbb{Q}$ the field of natural numbers, $\mathbb{A}$ the field of real algebraic numbers, $\mathbb{R}$ the field of real numbers, and $\mathbb{C}$ the field of complex numbers.

When discussing the background theory, we will try to keep results as generic as possible, so will let $\mathbb{k}$ denote a general field of characteristic zero and $\mathbb{K}$ an algebraic closure of $\mathbb{k}$ (in general $\mathbb{k}$ will represent the integers or rationals, and $\mathbb{K}$ the algebraic, real or complex numbers).

We will consider $n \in \mathbb{N}$ ordered variables, $\mathbf{x} = x_1 \prec x_2 \prec \cdots \prec x_n$. We use $\Bbbk[\mathbf{x}]$ to denote the ring of polynomials in $x_1, \ldots, x_n$ with coefficients in $\Bbbk$. We also use the notation

$$\mathbb{P}_i := \Bbbk[x_1, \ldots, x_i]$$

for $i = 1, \ldots, n$, with $\mathbb{P}_0 := \Bbbk$. When working over $\mathbb{C}$ we will use z_j to denote the variables, splitting them into $z_j = x_j + y_j \mathrm{i}$.

Remark 2.1.
Unfortunately, there is no standard way of notating variable order in CAD research. Indeed, the three main systems for computing CADs we will discuss (Maple, Mathematica and Qepcad) are not identical in their inputs. As such, it can be confusing to compare variable orderings.

To try and defend against this confusion, whenever the theory of CAD is discussed, the variables (in italicised form) will be given in ascending order: $x_1 \prec x_2 \prec \cdots \prec x_n$. However, when discussing a CAD implementation the variables (in monospace form) may be given in the appropriate ordering for the algorithm discussed. So for variables $a \prec b \prec c$ the orderings would be:

- Maple [`RegularChains`]: `[c,b,a]`;
- Maple [`ProjectionCAD`]: `[c,b,a]`;
- Qepcad: `(a,b,c)`;
- Mathematica: `{a,b,c}`.

These implementations of cylindrical algebraic decomposition will be discussed in Section 2.11.

We make some standard definitions that exist in the literature.

Definition 2.1.
For a polynomial $f \in \Bbbk[\mathbf{x}]$, the **main variable**, denoted $\mathrm{mvar}(f)$, is the greatest, with respect to the ordering $\prec$, variable $v \in \{x_1, \ldots, x_n\}$ such that $\deg(f, v) > 0$.

The **level** of f, denoted $\mathrm{level}(f)$, is the integer k such that $\mathrm{mvar}(f) = x_k$.

For a polynomial f of level k and a point $\alpha \in \mathbb{K}^{k-1}$ we write $f(\alpha, x_k, \ldots, x_n)$ to denote the specialisation of f at α, producing a polynomial in $\mathbb{K}[x_k, \ldots, x_n]$.

Definition 2.2.
We can consider a polynomial $f \in \Bbbk[\mathbf{x}]$ as a univariate polynomial in $\mathrm{mvar}(f)$. We define the following properties.

The **main degree** of f, denoted $\mathrm{mdeg}(f)$, is $\deg(f, \mathrm{mvar}(f))$.

The **initial** of f, denoted $\mathrm{init}(f)$, is the leading coefficient of f.

The **trail** of f, denoted $\mathrm{trail}(f)$, is the trailing coefficient of f.

The **leading monomial** (or **rank**) of f is denoted $\mathrm{lm}(f)$ (or $\mathrm{rank}(f)$).

The **leading term** (or **head**) of f is denoted $\mathrm{lt}(f)$ (or $\mathrm{head}(f)$).

The **tail** of f, denoted $\mathrm{tail}(f)$, is f without its leading term (that is, $f - \mathrm{lt}(f)$).

Finally, the **separant** of f, denoted $\mathrm{sep}(f)$, is the partial derivative of f with respect to $\mathrm{mvar}(f)$.

Definition 2.3.
Let f be a polynomial in $\mathbb{Z}[x_1, \ldots, x_n]$. The **squarefree decomposition** of f is an expression

$$f = \prod_{i=1}^{m} f_i^i, \tag{2.1}$$

where the f_i are relatively prime and have no repeated factors. We say that f is **squarefree** if $m = 1$ in (2.1).

Definition 2.4.
A set A of polynomials in $\mathbb{Z}[x_1, \ldots, x_n]$ is a **squarefree basis** if the elements of A have positive degree and are primitive, squarefree, and pairwise relatively prime.

2.1.2 Polynomial Ideals

Definition 2.5.
Let F be a finite set of polynomials $\{f_1, \ldots, f_m\} \subset \Bbbk[\mathbf{x}]$. We use $\langle F \rangle$ to denote the **polynomial ideal** generated by F:

$$\langle F \rangle := \left\{ h \in \Bbbk[\mathbf{x}] \;\middle|\; \exists g_i \in \Bbbk[\mathbf{x}] \text{ s.t. } h = \sum_{i=1}^{m} g_i f_i \right\}.$$

Definition 2.6.
The **zero set** or **algebraic variety** of F, denoted $\mathbf{V}(F)$, is defined to be all points in $\mathbb{K}^n$ such that all $f_i \in F$ vanish. If F is a singleton, say $F = \{f\}$, then we omit the set brackets, writing simply $\mathbf{V}(F)$. Note that clearly $\mathbf{V}(F)$ is equal to $\mathbf{V}(\langle F \rangle)$.

2.2 Cylindrical Algebraic Decomposition

The concept of a cylindrical algebraic decomposition was created by Collins in 1973 and introduced in [Col75] as a concept to tackle quantifier elimination over real closed fields.

2.2.1 Definition of Cylindrical Algebraic Decomposition

To deconstruct Collins' definition we will introduce some terminology and notation to make it more transparent (emulating [CMA82]). These definitions will be stated over $\mathbb{Q}$ and $\mathbb{R}$ but will extend to general $\Bbbk$ and $\mathbb{K}$ quite easily.

Definition 2.7.
We call a non-empty subset R of $\mathbb{R}^n$ a **region** of $\mathbb{R}^n$. Over such an R we define the **cylinder over** R, denoted $Z(R)$, to be $R \times \mathbb{R}$. We call a region of $\mathbb{R}^n$ an i**-cell**, $0 \leq i \leq n$, if it is homeomorphic to $\mathbb{R}^i$.

For any subset $X \subseteq \mathbb{R}^n$, a **decomposition** of X is a finite partition of X into (disjoint) regions.

Definition 2.8.
Let f be a continuous, real-valued function on $R \subseteq \mathbb{R}^n$. The f**-section** of $Z(R)$ is the set of points:

$$\left\{(\alpha, b) \in \mathbb{R}^{n+1} \;\middle|\; \alpha \in R,\ f(\alpha) = b\right\}$$

and we call any set of this form a **section**.

Let f_1 and f_2 be continuous, real-valued functions on R such that $f_1 < f_2$ (allowing the constant functions $f_1 = -\infty$ and $f_2 = +\infty$ if necessary). The (f_1, f_2)**-sector** of $Z(R)$ is the set of points:

$$\left\{(\alpha, b) \in \mathbb{R}^{n+1} \;\middle|\; \alpha \in R,\ f_1(\alpha) < b < f_2(\alpha)\right\}.$$

and we call any set of this form a **sector**.

Note that if the region R is an i-cell, then any section of $Z(R)$ will also be an i-cell and any sector of $Z(R)$ will be an $(i+1)$-cell.

Example 2.1.
We can see in Figure 2.1 a stack constructed over the interval (a, b). The three graphs separate the cylinder over (a, b) into four 2-dimensional cells (the sectors of the functions) and three 1-dimensional cells (the sections of the functions). Additionally, the cylinders

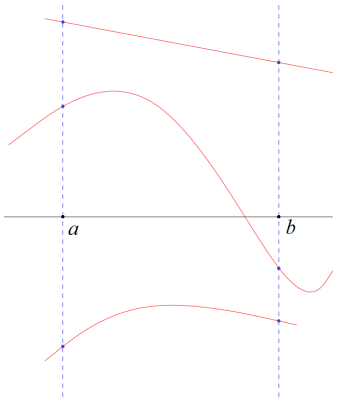


Figure 2.1: Stack over an interval

over the points a and b have each been decomposed into four 1-dimensional cells and three 0-dimensional cells.

Definition 2.9.
For a collection of continuous, real-valued functions $f_1 < f_2 < \cdots < f_k$ $(k \geq 0)$ defined on a region R there is a natural decomposition of $Z(R)$ into the following:

- The f_i-sections of $Z(R)$ for $1 \leq i \leq k$;
- The (f_i, f_{i+1})-sectors of $Z(R)$ for $0 \leq i \leq k$, where $f_0 = -\infty$ and $f_{k+1} = +\infty$.

Such a decomposition is called a **stack over** R, or an $(f_1, f_2, \ldots, f_k)$**-stack over** R.

Related to the concept of a stack is that of a delineable polynomial.

Definition 2.10.
For $f \in \mathbb{Q}[\mathbf{x}]$ and $R \subset \mathbb{R}^{n-1}$ we say that f is **delineable** on R if $V(f) \cap Z(R)$ consists of k disjoint sections of $Z(R)$, for some $k \geq 0$.

A delineable polynomial therefore gives rise to a natural stack over R, determined by the continuous functions whose graphs make up $V(f) \cap Z(R)$. We denote this stack $S(f, R)$ and talk of it consisting of the f**-sections** of $Z(R)$.

We now define the key concept of cylindricity in two ways. The first was the original definition given in [Col75] whilst the second has been used in more recent papers [CMXY09] and offers an alternative perspective. When discussing algebraic decompositions (Definition 2.13) the definitions are, in fact, equivalent.

Definition 2.11.
A decomposition $\mathcal{D}$ of $\mathbb{R}^n$ is said to be **cylindrical** if:

- $n = 1$ and $\mathcal{D}$ is a stack over the singleton set $(\mathbb{R}^0)$; or
- $n > 1$ and there is a cylindrical decomposition $\mathcal{D}'$ of $\mathbb{R}^{n-1}$ such that for each region R' of $\mathcal{D}'$, some subset of $\mathcal{D}$ is a stack over R'.

Such a $\mathcal{D}'$ is unique for a given $\mathcal{D}$ and is called the **induced (cylindrical) decomposition**. We, conversely, say that $\mathcal{D}$ is an **extension** of $\mathcal{D}'$.

Definition 2.12.
A decomposition $\mathcal{D}$ of $\mathbb{R}^n$ is said to be **cylindrical** if, for any pair of cells $D_i, D_j \in \mathcal{D}$ and any $1 \leq k \leq n$, the canonical projections to $\mathbb{R}^k$, $\pi_k(D_i)$ and $\pi_k(D_j)$, are identical or disjoint.

Definition 2.13.
A **semi-algebraic set** is one that can be written as a finite combination of unions, intersections, and complements of sets of the form:

$$\{\mathbf{x} \in \mathbb{R}^n \mid f(\mathbf{x}) = 0 \ \wedge \ g(\mathbf{x}) > 0\}$$

for polynomials $f, g \in \mathbb{Q}[\mathbf{x}]$.

A decomposition of $\mathbb{R}^n$ is called **algebraic** if each of its regions is a semi-algebraic set.

Remark 2.2.
Definitions 2.11 and 2.12 assume an underlying fixed variable ordering for the decomposition to be cylindrical with respect to. It may be possible to consider the idea of semi-monotone sets [BGV13] (which are convex with respect to all coordinate directions) and generalise to produce cells that are cylindrical with respect to multiple variables at once.

The following result follows from the existence of a quantifier elimination method for real closed fields, as first discovered in [Tar51].

Theorem 2.1 ([Tar51])**.**
A subset of $\mathbb{R}^n$ is semi-algebraic if and only if it is **definable***; that is, it equals the solution set of some standard formula Φ.*

There is a strong link between delineability and semi-algebraicity, as shown in the following theorem.

Theorem 2.2 ([Col75, CMA82])**.**
Let $n \geq 2$ and $f \in \Bbbk[\mathbf{x}]$ a delineable polynomial on a semi-algebraic region $R \subset \mathbb{K}^{n-1}$. Then the stack $S(f, R)$ is algebraic.

With the concepts described above, the definition of a cylindrical algebraic decomposition is straightforward.

Definition 2.14 ([CMA82])**.**
A **cylindrical algebraic decomposition (CAD) of** $\mathbb{R}^n$ is a decomposition of $\mathbb{R}^n$ that is both cylindrical and algebraic.

For the cells of a CAD we define an index.

Definition 2.15.
Let $\mathcal{D}$ be a cylindrical algebraic decomposition of $\mathbb{R}^n$. We define the **index** of a cell S of $\mathcal{D}$ to be a list of integers $[\![i_1, \ldots, i_n]\!]$ defined recursively as follows.

- If $n = 1$ then $\mathcal{D}$ consists of intervals and points. List the cells in increasing order so that the smallest is the 1-cell with $-\infty$ as its left-endpoint, the next cell is the 0-cell immediately to its right on the real line, and so forth. With this ordering, the smallest cell has index $[\![1]\!]$, the next cell has index $[\![2]\!]$, and so forth.
- If $n > 1$ then let $\mathcal{D}'$ be the induced cylindrical decomposition (Definition 2.11) of $\mathbb{K}^{n-1}$. Then a cell $D \in \mathcal{D}$ is an element of a stack over a cell $D' \in \mathcal{D}'$. Let $[\![i_1, \ldots, i_{n-1}]\!]$ be the index of D'. Number the cells of the stack over D' from bottom to top (that is, the bottommost cell is the n-cell with $-\infty$ as the left-endpoint for x_n). Then if D is the j^{th} cell of the stack its index is defined to be $[\![i_1, \ldots, i_{n-1}, j]\!]$.

It is worth noting that the dimension of cell is then equal to the sum of the parities of its indices; for a cell D with index $[\![i_1, \ldots, i_n]\!]$ we have

$$\dim(D) = \sum_{j=1}^{n} (\ i_j \bmod 2).$$

It is also clear that a CAD will always have an odd number of cells (this is true for all its induced CADs too).

We now to define the concept of invariance over a cell.

Definition 2.16.
Let $f \in \mathbb{Q}[\mathbf{x}]$ and R a region of $\mathbb{R}^n$. We say that f is **(sign)-invariant on** R and R is f**-invariant** if either:

- $f(\alpha) > 0$ for all $\alpha \in R$;
- $f(\alpha) = 0$ for all $\alpha \in R$; or
- $f(\alpha) < 0$ for all $\alpha \in R$.

Let $F \subset \mathbb{Q}[\mathbf{x}]$. Then R is **F-invariant** if every polynomial in F is invariant on R. A decomposition of $\mathbb{R}^n$ is **F-invariant** if every cell is F-invariant.

The following is the key result concerning invariance over stacks generated by a delineable polynomial which underpins many proofs regarding projection-based CAD.

Theorem 2.3 ([Col75, CMA82])**.**
Let $n \geq 2$, $F \subset \Bbbk[\mathbf{x}]$, and R a region of $\mathbb{K}^{n-1}$. Suppose each $f \in F$ is delineable on R and that $h = \prod_{f \in F} f$ is delineable on R. Then $S(h, R)$ is F-invariant.

2.2.2 Motivating Application: Quantifier Elimination

Quantifier Elimination was the original motivation of CAD, and is a well-established problem from mathematical logic. We recall some definitions relating to the decision theory of real closed fields.

Definition 2.17.
A **standard atomic formula** is a formula of one of the following six types:

$$f(\mathbf{x}) = 0, f(\mathbf{x}) > 0, f(\mathbf{x}) < 0, f(\mathbf{x}) \neq 0, f(\mathbf{x}) \geq 0, f(\mathbf{x}) \leq 0,$$

for some polynomial $f \in \Bbbk[\mathbf{x}]$.

A **standard formula** is any formula which can be constructed from standard atomic formulae using propositional connectives ($\neg$, $\wedge$, $\vee$, $\rightarrow$, $\leftrightarrow$) and quantifiers on variables ($\exists\ x_i$, $\forall\ x_i$).

Definition 2.18.
A **quantifier free formula** (or **QFF**) is a standard formula that does not involve any quantifiers on variables.

A **standard prenex formula**, or **Tarski formula**, is a standard formula which has the form

$$\Phi := (Q_k x_k)(Q_{k+1} x_{k+1}) \cdots (Q_n x_n) \varphi(x_1, \ldots, x_n)$$

where $\varphi(x_1, \ldots, x_n)$ is a quantifier-free standard formula of $\mathbf{x}$, the value of k is between 0 and n, and each Q_i is a universal or existential quantifier. We say that $x_1, \ldots, x_{k-1}$

are **free variables** with respect to Φ, and $x_k, \ldots, x_n$ are **bound variables** with respect to Φ.

Problem 2.1 (Quantifier Elimination)**.**
Let Φ be a standard prenex formula over $\mathbb{k}$ of the form:

$$\Phi := (Q_k x_k)(Q_{k+1} x_{k+1}) \cdots (Q_n x_n)\varphi(x_1, \ldots, x_n).$$

The **Quantifier Elimination Problem** is to find a quantifier free formula in the free variables, $\Psi(x_1, \ldots, x_{k-1})$, which is **equivalent** to Φ:

$$(\forall x_1)(\forall x_2) \cdots (\forall x_{k-1})\big[\Phi = \Psi\big].$$

In [Tar51], it was shown that the theory of real closed fields allows an algorithmic solution to Problem 2.1. In doing so, Tarski showed that the theory of real closed fields is complete and decidable. This proves the important result that definability and semi-algebraicity are equivalent properties (see Theorem 2.1).

Although Tarski proved that Problem 2.1 has an algorithmic solution, his method has non-elementary complexity in the number of variables. This means that there is no finite tower of exponentials, such as:

$$2^{2^{\cdot^{\cdot^{\cdot^{2^n}}}}}$$

sufficient to describe the complexity of the algorithm.

Cylindrical algebraic decomposition [Col75] gave a more efficient method to eliminate quantifiers[1], although (as discussed in Section 2.6) it is still limited by doubly-exponential complexity [DH88, BD07]. By constructing a sign-invariant CAD of the polynomials for a quantifier elimination problem, the evaluation of Φ on the induced CAD of $\mathbb{R}^{k-1}$ can identify all cells on which Φ holds. Taking the conjunction of the descriptions of these valid cells gives a quantifier free formula logically equivalent to Φ.

[1] At the same time as Collins published his work on CAD, a quantifier elimination procedure was given in [Wüt74].

2.3 Projection and Lifting Cylindrical Algebraic Decomposition

We now discuss the original algorithm provided by Collins in [Col75] (and also detailed in [CMA82]), along with the many extensions to its theory and implementation.

2.3.1 Collins' Algorithm

Informally, the algorithm has two main stages: projection and lifting. The projection phase produces a sequence of sets of polynomials in $\mathbb{P}_{n-1}$, $\mathbb{P}_{n-2}$ and so forth. Once the projection phase produces polynomials in $\mathbb{P}_1$ (univariate in x_1) a decomposition of $\mathbb{R}^1$ is produced from these. The lifting phase then takes a decomposition of $\mathbb{R}^1$ and produces, using the projection polynomials, a decomposition of $\mathbb{R}^2$. Repeating this we eventually produce an F-invariant cylindrical algebraic decomposition of $\mathbb{R}^n$.

Definition 2.19.
We refer to any cylindrical algebraic decomposition algorithm that utilises a projection and lifting approach to construction as a **projection and lifting CAD algorithm**. We also refer to the output of such an algorithm as a **PL-CAD**[2].

Projection

We need two more definitions before defining Collins' projection operator.

Definition 2.20.
For $f \in \mathbb{k}[\mathbf{x}]$ and $R \subset \mathbb{K}^{n-1}$ we say f is **identically zero** on R if $f(\alpha, x_n)$ is equal to zero for all $\alpha \in R$.

For a set of polynomials $F \subset \mathbb{k}[\mathbf{x}]$ and a set $R \subset \mathbb{K}^{n-1}$ we define the **non-zero product of F on R**, F_R, to be the product of all $f \in F$ that are not identically zero on R. If all elements of F are identically zero on R then $F_R := 1 \in \mathbb{k}[\mathbf{x}]$.

Definition 2.21.
For $f \in \mathbb{k}[\mathbf{x}]$ the **reductum** of f, written $\text{red}(f)$, is simply $\text{tail}(f)$. Furthermore, for $k \geq 0$, we define the **k^{th}-reductum** recursively:

$$\begin{aligned} \text{red}^0(f) &:= f; \\ \text{red}^{k+1}(f) &:= \text{tail}(\text{red}^k(f)). \end{aligned}$$

[2] A list of CAD acronyms is given in Appendix D for easy reference.

The **reducia set** of f, denoted $\mathrm{RED}(f)$ is the set of non-zero reducia of f:

$$\mathrm{RED}(f) := \{\mathrm{red}^k(f) \mid 0 \leq k \leq \deg(f),\ \mathrm{red}^k(f) \neq 0\}.$$

We now describe the original projection operator, ${}_{\mathbf{C}}\mathbf{P}$, which computes the principal subresultant coefficient set, PSC, for various reducia. The PSC defines the interaction of two polynomials in great detail, and culminates in the resultant of the polynomials.

Definition 2.22 ([Col75])**.**
Let $F = \{f_1, \ldots, f_m\} \subset \mathbb{Q}[x_1, \ldots, x_n]$. For each $f_i \in F$ let $R_i := \mathrm{RED}(f_i)$. We define the two sub-projection sets:

$$\begin{aligned}
{}_{\mathbf{C}}\mathbf{P}_1(F) &:= \bigcup_{i=1}^{m} \bigcup_{g_i \in R_i} \big(\{\mathrm{init}(g_i)\} \cup \mathrm{PSC}(g_i, \mathrm{sep}(g_i))\big); \\
{}_{\mathbf{C}}\mathbf{P}_2(F) &:= \bigcup_{1 \leq i < j \leq m} \bigcup_{\substack{g_i \in R_i \\ g_j \in R_j}} \mathrm{PSC}(g_i, g_j).
\end{aligned}$$

We then define the **(Collins) projection set**, ${}_{\mathbf{C}}\mathbf{P}(F)$, as:

$${}_{\mathbf{C}}\mathbf{P}(F) := {}_{\mathbf{C}}\mathbf{P}_1(F) \cup {}_{\mathbf{C}}\mathbf{P}_2(F).$$

We now state the key theorems necessary for the use of ${}_{\mathbf{C}}\mathbf{P}$.

Theorem 2.4 ([Col75, CMA82])**.**
Let $n \geq 2$ and $F \subset \mathbf{k}[x_1, \ldots, x_n]$. Let R be a ${}_{\mathbf{C}}\mathbf{P}(F)$-invariant region in $\mathbb{K}^{n-1}$. Then:

- *Every $f \in F$ is either delineable or identically zero on R;*
- *The nonzero-product of F on R, F_R, is delineable on R.*

Therefore, there exists an algebraic, F-invariant stack over R, namely $S(F_R, R)$.

Theorem 2.5 ([Col75, CMA82])**.**
The projection operator ${}_{\mathbf{C}}\mathbf{P}$ is a valid projection operator, that is, it can be used to produce an F-invariant CAD.

Base Case and Lifting

Let F^* equal ${}_{\mathbf{C}}\mathbf{P}^{(n-1)}(F)$. Construct the set of relatively prime, distinct, irreducible factors of F^*. The real roots of these factors will be the 0-cells of $\mathcal{D}^*$ and the open

Algorithm 2.1: `SplitR(F)`: 1-dimensional space decomposition algorithm.

Input : A set of univariate polynomials, F^*.
Output: A decomposition, $\mathcal{D}$, of $\mathbb{R}$ with each cell represented as a list consisting of a cell index and a sample point.

$\mathcal{D}^* \leftarrow [\,]$;
$f^* \rightarrow \prod_{f \in F^*} f$;
$r \leftarrow \text{roots}(f^*)$; $n \leftarrow |r|$; `// Compute roots of` f^*
if $n = 0$ **then**
    $\mathcal{D}^*.append([[\![1]\!], 0])$; `// no roots; construct trivial stack`
    return $\mathcal{D}^*$;
$\mathcal{D}^*.append([[\![1]\!], \texttt{SamplePoint}((-\infty, r[1]))])$; `// Initial interval`
$\mathcal{D}^*.append([[\![2]\!], r[1]])$;
for $i = 2, \ldots, n$ **do**
    $\mathcal{D}^*.append([[\![2i-1]\!], \texttt{SamplePoint}((r[i-1], r[i]))])$;
    $\mathcal{D}^*.append([[\![2i]\!], r[i]])$;
$\mathcal{D}^*.append([[\![2n+1]\!], \texttt{SamplePoint}((r[n], \infty))])$; `// Final interval`
return $\mathcal{D}^*$;

intervals defined by these roots will be the 1-cells of $\mathcal{D}^*$. This is described in Algorithm 2.1, where `SamplePoint` is a sub-algorithm that takes a (possibly infinite) interval and provides a rational sample point from that interval.

For lifting we need to construct cells over a given cylindrical algebraic decomposition according to the solutions of these $_{\mathbf{C}}\mathbf{P}$ sets. This is done by creating stacks over each cell using the $_{\mathbf{C}}\mathbf{P}$ polynomials and assigning cell indices and sample points appropriately. For implementation this requires careful treatment of algebraic numbers but this is not the focus of our research so is not detailed here. The algorithm `GenerateStack` executes this lifting stage and is described in Algorithm 2.2.

Complete Projection and Lifting Algorithm

We can combine the ideas of this section to produce Algorithm 2.3, which is the algorithm described in [Col75] and [CMA82]. The procedure `Proj` refers to an implementation of Collins' projection operator, `SplitR` is defined in Algorithm 2.1, and `GenerateStack` is defined in Algorithm 2.2.

Algorithm 2.2: `GenerateStack(F, x_k, D)`: Stack generation (lifting) algorithm.

Input : A set of k-variate polynomials, F; a variable to lift with respect to, x_k; a cell to lift over, D.
Output: A stack, S, of cells in $\mathbb{R}^k$ over D, with each cell represented as a list consisting of a cell index and a sample point.

$S \leftarrow [\,]$;
$I \leftarrow D$.`index`; $\alpha \leftarrow D$.`samplepoint`;
$f^*(x_k) \rightarrow \prod_{f \in F} f(\alpha, x_k)$; `// Specialise product at` α
$r \leftarrow \text{roots}(f^*)$; $n \leftarrow |r|$;
if $n = 0$ **then**
    $S.append([[\![I, 1]\!], (\alpha, 0)])$; `// No roots; construct trivial stack`
    return S;
$S.append([[\![I, 1]\!], (\alpha, \texttt{SamplePoint}((-\infty, r[1])))])$; `// Initial interval`
$S.append([[\![I, 2]\!], (\alpha, r[1])])$;
for $i = 2, \ldots, n$ **do**
    $S.append([[\![I, 2i-1]\!], (\alpha, \texttt{SamplePoint}((r[i-1], r[i])))])$;
    $S.append([[\![I, 2i]\!], (\alpha, r[i])])$;
$S.append([[\![I, 2n+1]\!], (\alpha, \texttt{SamplePoint}((r[n], \infty)))])$; `// Final interval`
return S;

Algorithm 2.3: `CAD(F, vars)`: Projection and Lifting-based CAD algorithm.

Input : A set of polynomials, F; an ordered list of variables, $vars = [x_1, \ldots, x_n]$.
Output: A CAD, $\mathcal{D}$, that is sign-invariant with respect to F.

$\mathcal{D} \leftarrow [\,]$;
$\mathcal{P} \leftarrow [\,]$;
$\mathcal{P}[1] \leftarrow F$;
for $i = 2, \ldots, n$ **do**
    $\mathcal{P}[i] = \texttt{Proj}(\mathcal{P}[i-1], x_{n-(i-2)})$; `// Projection phase`
$\mathcal{D}[1] \leftarrow \texttt{SplitR}(\mathcal{P}[n])$; `// Base case`
for $i = 2, \ldots, n$ **do**
    for $D \in \mathcal{D}[i-1]$ **do**
        $\mathcal{D}[i].append(\texttt{GenerateStack}(\mathcal{P}[n-i+1], x_i, D))$; `// Lifting phase`
return $\mathcal{D}[n]$;

2.4 Extensions to Collins' algorithm

Collins' method often provides a CAD that is much more complicated than necessary. There have been extensions to his algorithm which will be described briefly.

2.4.1 Alternative Projection Operators

One of the key areas of improvement has been in the projection operator $\mathbf{_C P}$. We present three well-documented projection operators: the Collins–Hong operator [Hon90], McCallum's operator [McC85, McC88] and the Brown–McCallum operator [Bro01]. We will also discuss a projection operator proposed by Lazard [Laz94] for which the original proof is flawed and so, as yet, is unverified.

For all of the following operators let $F = \{f_1, \ldots, f_m\}$ be integral polynomials defined on variables $x_1, \ldots, x_n$. We use the standard assumptions that the elements of F are primitive, squarefree and pairwise relatively prime (which must be ensured to hold when implementing CAD algorithms).

Hong's Projection ([Hon90])

Definition 2.23.
The **Collins–Hong projection set**, which we shall denote $\mathbf{_{CH}P}(F)$, is defined as:

$$\mathbf{_{CH}P}(F) := \mathbf{_C P}_1(F) \cup \mathbf{_{CH}P}_2(F).$$

where the second component is defined as:

$$\mathbf{_{CH}P}_2(F) := \bigcup_{1 \le i < j \le m} \bigcup_{g_i \in R_i} \mathrm{PSC}(g_i, f_j).$$

The Collins–Hong projection operator is a subset of the Collins operator ($\mathbf{_C P}_2(F)$ also ranges over the reductum of f_j), and requires no additional conditions on the input. It should therefore always be used in place of Collins' operator.

McCallum's Projection ([McC85, McC98])

Definition 2.24.
The **McCallum projection set**, which we shall denote $\mathbf{_M P}(F)$, is defined as follows:

$$\mathbf{_M P}(F) := \mathbf{_M P}_1(F) \cup \mathbf{_M P}_2(F) \cup \mathbf{_M P}_3(F)$$

with the sub-projections defined as follows:

$$
\begin{aligned}
{}_{\mathbf{M}}\mathbf{P}_1(F) &:= \bigcup_{i=1}^{m} \{\text{non-zero coefficients of } f_i \in \mathbb{R}[x_n]\} \\
{}_{\mathbf{M}}\mathbf{P}_2(F) &:= \{\text{disc}_{x_n}(f_i) \mid \text{disc}_{x_n}(f_i) \neq 0,\ i = 1, \ldots, m\} \\
{}_{\mathbf{M}}\mathbf{P}_3(F) &:= \{\text{res}_{x_n}(f_i, f_j) \mid \text{res}_{x_n}(f_i, f_j) \neq 0,\ i, j = 1, \ldots, m,\ i \neq j\}
\end{aligned}
$$

The McCallum projection is a subset of the Collins operator, removing redundant polynomials and is simple to implement. However, McCallum proved that lifting over a sign-invariant cylindrical algebraic decomposition with this projection set is not sufficient to guarantee sign-invariance. The stronger idea of an **order-invariant** cylindrical algebraic decomposition is introduced.

Definition 2.25 ([McC85, McC98])**.**
Let $f \in \mathbb{Q}[\mathbf{x}]$ and R a region of $\mathbb{R}^n$. We say that f is **order-invariant on** R and R is f**-order-invariant** if either:

1. $f(\alpha) \neq 0$ for all $\alpha \in R$; or
2. $f(\alpha) = 0$ and vanishes to the same **order** for all $\alpha \in R$: the **order** of f at α is the least $k \in \mathbb{N}$ such that some partial derivative of f of order k does not vanish at α.

Let $F \subset \mathbb{Q}[\mathbf{x}]$. Then R is F**-order-invariant** if every polynomial in F is order-invariant on R. A decomposition of $\mathbb{R}^n$ is F**-order-invariant** if every cell is F-order-invariant.

Remark 2.3.
For $n \leq 2$, sign-invariance implies order-invariance [McC88].

For McCallum's operator to be valid we must ensure that the polynomials involved do not vanish identically on cells of positive dimension.

Definition 2.26 ([McC85, McC98])**.**
A set, F, of polynomials is said to be **well-oriented** if no element of a basis for F vanishes identically on any cell of positive dimension, and the same condition holds recursively for ${}_{\mathbf{M}}\mathbf{P}(F)$.

Theorem 2.6 ([McC85, McC98])**.**
Let F be a finite, square-free basis of n-variate integral polynomials. Let S be a connected

Algorithm 2.4: `CADW(F, vars)`: Projection and Lifting-based CAD algorithm using McCallum's projection operator as specified in [McC98].

Input : A set of polynomials, F; an ordered list of variables, $vars = [x_1, \ldots, x_n]$.
Output: A CAD, $\mathcal{D}$, that is order-invariant with respect to F, or **FAIL** if F is not well-oriented.

```
1  D ← [ ];
2  P ← [ ];
3  P[1] ← F;
4  for i = 2, ..., n do
5      P[i] = MProj(P[i − 1], x_{n−(i−2)});                    // Projection phase
6  D[1] ← SplitR(P[n]);                                        // Base case
7  for i = 2, ..., n do
8      for D ∈ D[i − 1] do
9          i ← D.index;  α ← D.samplepoint;
10         if dim(D) > 0 and ∃ h ∈ P[n − i + 1] s.t. h(α, x_i) ≡ 0 then
11             return FAIL;                                    // Input not well-oriented
12         if dim(D) = 0 then
13             Dpolys ← Delineating Set;
14         D[i].append(GenerateStack(P[n − i + 1] ∪ DPolys, x_i, D));   // Lifting
           phase
15 return D[n];
```

submanifold of $\mathbb{R}^{n-1}$. *Suppose each element of* F *is not identically zero on* S *and each element of* ${}_{\mathbf{M}}\mathbf{P}(F)$ *is order-invariant on* S.

Then each element of F *is analytically delineable on* S *[McC98, §3], the sections of* F *over* S *are pairwise disjoint, and each element of* F *is order-invariant in every section of* A *over* S.

Therefore ${}_{\mathbf{M}}\mathbf{P}$ can be used for a set of well-oriented polynomials. Note that sets of polynomials are generally well-oriented: in [McC85] a discussion is given to show that well-orientedness is likely. However, as shown by various examples, it can still prevent CAD construction.

The full construction of a CAD by McCallum's projection operator is given in Algorithm 2.4, as discussed in [McC98]. Well-orientedness prevents nullification on positive dimensional cells; nullification on a zero-dimensional cell is dealt with through delineating polynomials on line 13 (described in [McC98]).

Brown-McCallum's Projection ([Bro01])

Definition 2.27.
The **Brown–McCallum projection set**, which we shall denote ${}_{\mathbf{BM}}\mathbf{P}(F)$ is defined as follows:

$$ {}_{\mathbf{BM}}\mathbf{P}(F) := {}_{\mathbf{BM}}\mathbf{P}_1(F) \cup {}_{\mathbf{M}}\mathbf{P}_2(F) \cup {}_{\mathbf{M}}\mathbf{P}_3(F) $$

with the first component defined as:

$$ {}_{\mathbf{BM}}\mathbf{P}(F) := \{\text{init}(f_i) \mid i = 1, \ldots, m\}. $$

As with ${}_{\mathbf{M}}\mathbf{P}$, we need the polynomials to be well-oriented for ${}_{\mathbf{BM}}\mathbf{P}$ to be a valid projection operator. However, there is the added condition that any points where a polynomial vanishes must also be manually included into the cylindrical algebraic decomposition. This process of identifying these points takes significant time, but Brown argues that using ${}_{\mathbf{BM}}\mathbf{P}$ is still cheaper than ${}_{\mathbf{M}}\mathbf{P}$, demonstrated by its implementation in QEPCAD-B.

Lazard's Postulated Projection ([Laz94])

Definition 2.28.
The **Lazard projection set**, which we shall denote ${}_{\mathbf{L}}\mathbf{P}(F)$ is defined as follows:

$$ {}_{\mathbf{L}}\mathbf{P}(F) := {}_{\mathbf{BM}}\mathbf{P}(F) \cup {}_{\mathbf{L}}\mathbf{P}_4(F) $$

with the additional projection set defined as:

$$ {}_{\mathbf{L}}\mathbf{P}_4(F) := \{\text{trail}(f_i) \mid i = 1, \ldots, m\}. $$

Note that the Lazard projection operator is a subset of McCallum's projection operator and a superset of the Brown-McCallum projection operator. The use of this operator would still require well-oriented polynomials but would not need vanishing points to be added. Therefore it could replace the ${}_{\mathbf{M}}\mathbf{P}$ operator, and depending on the number of vanishing points could prove more efficient than ${}_{\mathbf{BM}}\mathbf{P}$.

Whilst Lazard initially presented a proof of the validity of ${}_{\mathbf{L}}\mathbf{P}$ it was later found to be flawed. Recent progress on this work by McCallum and Hong has been submitted for publication [McC14].

Other Work

There has recently been progress in improving the projection operator [HJX12, HDX14, Str14]. In [HJX12] a projection operator is given to help find when, with respect to a single parameter, a given polynomial is uniformly positive. This operator is a subset (often strict) of the Brown's projection operator. In [HDX14] Brown's projection operator is computed with respect to multiple variable orders and intersects them through gcd computation to simplify the projection. This approach guarantees a sample point in each open connected component. In [Str14] the projection operator is adapted to each particular cell (producing a **local projection set**). This not only simplifies the number of cells produced, by using the Boolean structure and signature of the problem on each indiviual cell, but can also avoid irrelevant failure due to a lack of well-orientedness (Definition 2.26).

2.4.2 Partial CAD

In [CH91] the idea of a partial CAD was introduced. For a given Quantifier Elimination problem, instead of lifting a whole CAD, partial CAD constructs stacks over cells in order and, wherever possible, the lifting is truncated using two main ideas.

Quantifiers: Consider the sentence $(\exists\, x)(\exists\, y)\varphi(x,y)$. Then when lifting from $\mathbb{R}$ to $\mathbb{R}^2$ the algorithm would stop as soon as it found a cell satisfying $(\exists\, y)\varphi(x,y)$, returning **TRUE**. Alternatively, if the sentence was $(\forall\, x)(\exists\, y)\varphi(x,y)$, the algorithm would stop as soon as any cell is found in which $\neg(\exists\, y)\varphi(x,y)$ and return **FALSE**.

Boolean connectives: Consider the sentence $(\exists\, x)(\exists\, y)\varphi(x,y)$ where $\varphi(x,y) = \varphi_1(x) \wedge \varphi_2(x,y)$, where φ_i are quantifier-free formulae. Then we can evaluate $\varphi_1(x)$ on a cell, D' of the $\mathbb{R}^1$ CAD, $\mathcal{D}'$. If false, then $\varphi(x,y)$ must be false for all y and so there is no need to construct a stack over D'. Alternatively, if $\varphi(x,y) = \varphi_1(x) \vee \varphi_2(x,y)$ and $\varphi_1(x)$ is true on D' then there is no need to construct a stack over D'.

Whilst using partial CAD there is also the consideration of which order to choose the cells to lift over, which can clearly affect the time taken: constructing a lone cell that satisfies the formula first could prevent the construction of doubly-exponential cells that do not satisfy the formula. The authors of [CH91] suggest a variety of choices dependent on the type of problem (robot motion planning, systems of strict inequalities, termination proofs), providing experimental justification.

There has also been work on adapting the projection operator within partial CAD [SS03]. The authors of [SS03] introduce a generic projection operator, which is placed

between Collins' and Brown's operators and considers solutions only within a region defined by assumptions on the parameters. This approach is particularly well-suited for formulae with many parameters and polynomials of high degree.

2.4.3 Truth-Invariant CAD

In [Bro98], Brown introduced the idea of truth-invariance for a CAD. He gave the following definitions:

Definition 2.29 ([Bro98])**.**
Let $\mathcal{A}$ and $\mathcal{B}$ be two CADs. We say $\mathcal{B}$ is **simpler** than $\mathcal{A}$ if $\mathcal{A}$ is a refinement of $\mathcal{B}$, i.e. each cell in $\mathcal{B}$ is the union of some cells of $\mathcal{A}$, and $\mathcal{A}$ and $\mathcal{B}$ are not equal.

Given a formula φ from the elementary theory of real closed fields, we say a CAD is **truth-invariant** with respect to the input formula if in each cell of the decomposition the formula is either identically true or identically false.

Brown starts by looking at cells on the top level of a CAD of free variable space. Let $x_1, \ldots, x_k$ be the free variables of a quantified formula Φ, with quantifier free part $\varphi(x_1, \ldots, x_n)$. Then if none of the sections of a polynomial of level k form the boundary between a true and false region of $\mathbb{R}^k$ then it can be ignored when constructing a truth-invariant CAD. As only level k polynomials are potentially being discarded, no inter-stack boundaries will be removed, so only intra-stack adjacencies need to be considered.

When considering simplifying a CAD at lower levels the following definition is important.

Definition 2.30 ([Bro98])**.**
Let $C \in \mathcal{D}$ be an i-level section cell of a φ-truth-invariant cylindrical algebraic decomposition, and let B and D correspond to the neighbouring cells within the stack containing C. Suppose all polynomials of level i and greater are delineable over the union $B \cup C \cup D$. We say that C is a **truth-boundary cell** (or more specifically an **i-level truth-boundary cell**) if there exists a triple of cells (B', C', D') such that:

- B', C', and D' lie in the stacks over B, C, and D, respectively;
- $B' \cup C' \cup D'$ is a cell in the stack over $B \cup C \cup D$; and
- B', C', and D' do not all have the same truth value for φ.

Consider a quantified formula Φ, with quantifier free part $\varphi(x_1, \ldots, x_n)$. Brown provides an algorithm to create a truth-invariant CAD with respect to φ (called `SIMPLECAD`).

This takes as input the projection factors, P, and a CAD, $\mathcal{D}$, which is sign-invariant with respect to P (and therefore truth invariant with respect to φ). The output is a subset $\bar{P} \subseteq P$ (closed under projection), and a $\bar{P}$-sign-invariant CAD $\bar{\mathcal{D}}$ that is still truth invariant with respect to φ.

Initialising $\bar{P} := \varnothing$ and $\bar{\mathcal{D}} := \mathcal{D}$, Brown produces his truth-invariant CAD iteratively. Starting at the highest level and working down, at loop i:

1. add the projection of its elements to $\bar{P}$;
2. construct the set of all i-level truth boundary cells in $\bar{\mathcal{D}}$ that are not sections of $\bar{P}$;
3. for each cell in this set, take all i-level polynomials in P which are zero on that cell.
4. construct a minimal hitting set for these polynomials and add to $\bar{P}$;
5. simplify $\bar{\mathcal{D}}$ according to the new definition of $\bar{P}$.

The combination of the initial removal of level k polynomials that do not form boundaries between true and false cells, and then using `SIMPLECAD`, is implemented within QEPCAD-B. Brown shows that it can construct substantially simpler CADs (which also results in a simpler quantifier-free formulae).

2.4.4 Equational Constraints

In [Col98] the idea of equational constraints was first introduced. The idea was later expanded upon [McC99, McC01, BM05].

Definition 2.31.
For a given quantifier elimination problem Φ, a **constraint** is an atomic formula which is logically implied by the quantifier free part, φ, of Φ. If such a constraint is an equation we call it an **equational constraint**.

If $\varphi := (f = 0) \wedge \hat{\varphi}$ then f is an equational constraint, and we say that f is an **explicit equational constraint** of φ. Alternatively, if $\varphi := (f_1 = 0) \vee (f_2 = 0)$ then the equation $f_1 f_2 = 0$ is an equational constraint, and we say that $f_1 f_2 = 0$ is an **implicit equational constraint** of φ.

The idea behind using equational constraints to simplify the projection operator is that we only need to be concerned with the behaviour of polynomials whilst the equational constraint is satisfied. Therefore, if $f = 0$ is an equational constraint and g

is any other polynomial in φ, then the behaviour of g when f is non-zero does not affect the behaviour of φ. Hence, instead of including the coefficients and discriminant of g or its resultant with any polynomial that is not f in the first projection set, we just need to include $\text{res}_{x_n}(f, g)$. This is given formally in Definition 2.32.

Let f be an equational constraint polynomial for Φ. Let A be the set of irreducible factors of all polynomials in Φ with positive degree in x_n. Let E be the subset of A containing irreducible factors of f.

Definition 2.32 ([McC99])**.**
The **restricted projection** (or **equational constraint projection**) of A relative to E, ${}_{\mathbf{M}}\mathbf{P}_E(A)$ is defined to be:

$$ {}_{\mathbf{M}}\mathbf{P}_E(A) := {}_{\mathbf{M}}\mathbf{P}(E) \cup \{\text{res}_{x_n}(f, g) \mid f \in E, g \in A, g \notin E\}. $$

The following key theorem from [McC99] shows that if ${}_{\mathbf{M}}\mathbf{P}_E(A)$ is used for the first projection and E is used for the final lifting the produced CAD is sufficient to solve Φ.

Theorem 2.7 ([McC99])**.**
Let A be a set of pairwise relatively prime and irreducible integral polynomials of positive degree in x_n ($n \geq 2$). Let E be a subset of A. Let S be a connected submanifold of $\mathbb{R}^{n-1}$. Suppose that each element of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ is order-invariant in S. Then each element of E either vanishes identically on S or is analytic delineable on S, the sections over S of the elements of E which do not vanish identically on S are pairwise disjoint, each element of E is order-invariant in every such section, and each element of A not in E is sign-invariant in every such section.

Note that the fact the elements of A are sign-invariant (and not order-invariant) means that ${}_{\mathbf{M}}\mathbf{P}_E(A)$ cannot be used repeatedly, unless $n \leq 3$ (recall Remark 2.3).

In [McC01] the author defines the **semi-restricted projection** ${}_{\mathbf{M}}\mathbf{P}^*_E(A)$ of A relative to E to be

$$ {}_{\mathbf{M}}\mathbf{P}^*_E(A) := P_E(A) \cup \{\text{disc}_{x_n}(g) \mid g \in A, g \notin E\}. $$

This set guarantees order-invariance of $g \in A$ in sections of f over cells and so could be used repeatedly throughout the whole algorithm.

The author also notes how multiple equational constraints provide constraints for lower levels: if f_1 and f_2 are both equational constraints, then so is their resultant. In [BM05] the authors take this further and describe an algorithm that computes a CAD reliant on the variety $V(f, g)$ rather than the separate polynomials. The authors point

out that this is the first step towards a theory of CAD which is defined on systems of equations rather than individual polynomials.

The theory of equational constraints and truth-invariant CADs will be generalised in Chapter 3 into the idea of truth table invariant CADs, which allow for the logical structure of formulae to be exploited even further.

Remark 2.4.
Theorem 2.7 allows for a simplified lifting operator at the final lifting stage. As the non-equational constraints, A, are guaranteed to be sign-invariant on the sections of the equational constraint, the final lift need only be conducted with respect to E. This extension was introduced in [Eng13a, BDE$^+$14] and will be discussed in Chapter 3.

2.4.5 Solving Strict Inequalities

Given a problem involving only strict polynomial inequalities, any cells that satisfy the inequalities must necessarily be full dimensional. In [McC93] and later in [Str00] algorithms are given that only lift over full-dimensional cells at each stage of the algorithm. This idea will be revisited in Chapter 4.

A full-dimensional cell in a CAD is a product of open intervals, and so the sample points are from $\mathbb{Q}^n$. Not requiring the use of algebraic number computation increases the efficiency of the algorithm both in experimentation and theoretical complexity (discussed in Section 2.6).

2.4.6 Preconditioning for CAD

It is possible to precondition the input for a CAD algorithm to try to improve the efficiency.

In [BH91] the authors considered the use of Gröbner bases as a preconditioning technique for quantifier elimination by CAD. They show that it is often, but not always, beneficial to replace a conjunction of equalities by their Gröbner basis. This is investigated further in Chapter 6.

In [BG06] the author pre-processes the input formula for quantifier elimination. They substitute linear equational constraints to build a space of equivalent statements. They then use a grading function (which notes properties relating to the Boolean and quantifier structure) and search for a minimal formula.

In [BS10] the authors provide two methods for fast simplification of quantifier elimination problems, which are integrated into algorithms for quantifier elimination by both virtual substitution and cylindrical algebraic decomposition. Black box simplification

is conducted by considering the Boolean structure of the formula with respect to sign conditions[3]. White box simplification uses the polynomials themselves to deduce sign conditions (such as given $1 - x + y^2$ using $2x - 1 < 0$ to deduce $1 - x + y^2 > 0$).

2.5 Regular Chains Cylindrical Algebraic Decomposition

Until recent years, the only method of calculating a cylindrical algebraic decomposition was that given in [Col75]. In [CMXY09] a new method was described reliant on the theory of triangular decompositions and regular chains. This was later extended in [CM12] to provide an incremental (by polynomial) approach to building a cylindrical algebraic decomposition. These algorithms have been implemented in the `RegularChains` package for MAPLE; the former algorithm has been available, as `SemiAlgebraicTools[CylindricalAlgebraicDecompose]`, since MAPLE 16, and the latter will be freely available from the `RegularChains` research group website[4].

2.5.1 Triangular Decomposition

We begin by covering some of the key concepts in the theory of regular chains and triangular decompositions. This is a very deep subject and for a comprehensive discussion see [Maz05].

Definition 2.33.
For a set of polynomials $F \subset \Bbbk[\mathbf{x}]$ we define h_F to be the product of the initials of all polynomials in F. The **quasi-component** of F, denoted $\mathbf{W}(F)$, is defined to be

$$\mathbf{W}(F) := \mathbf{V}(F) \setminus \mathbf{V}(h_F).$$

For any $h \in \Bbbk[\mathbf{x}]$ we define $\mathbf{Z}(F, h)$ to be $\mathbf{W}(F) \setminus \mathbf{V}(h)$.

Definition 2.34.
Let $F \subset \Bbbk[\mathbf{x}]$ be a set of non-constant polynomials. We say F is a **triangular set** if the polynomials in F have pairwise disjoint main variables.

Let $\mathrm{mvar}(F)$ be the set of the main variables of the polynomials in F. A variable x is **algebraic** with respect to F if $x \in \mathrm{mvar}(F)$, and is otherwise **free**.

[3] This has been implemented, by Brown, into the SLFQ extension for QEPCAD-B: `http://www.usna.edu/CS/~qepcad/SLFQ/Home.html`

[4] `www.regularchains.org`

The sets $F_{<x}$ and $F_{>x}$ are defined to be all polynomials $f \in F$ such that $\text{mvar}(f) \prec x$ and $\text{mvar}(f) \succ x$, respectively. If $x \in \text{mvar}(F)$ we let F_x denote the unique polynomial in F such that $\text{mvar}(F_x) = x$.

Definition 2.35.
Let $h \in \Bbbk[\mathbf{x}]$ and $F \subset \Bbbk[\mathbf{x}]$ be a triangular set. The **iterated resultant** of h with respect to F, $\text{ires}(h, F)$, is defined as follows:

1. If $h \in \Bbbk$ or all variables in h are free with respect to F then $\text{ires}(h, F) := h$.
2. Otherwise, if x is the largest variable of h which is in $\text{mvar}(F)$ then

$$\text{ires}(h, F) := \text{ires}(r, F_{<x}), \quad \text{where} \quad r := \text{res}_x(h, F_x).$$

Definition 2.36.
Let $F \subset \Bbbk[\mathbf{x}]$ be a triangular set of polynomials. The **saturated ideal** of F, $\text{sat}(F)$ is defined to be $\langle 0 \rangle$ if $F = \varnothing$, otherwise:

$$\text{sat}(F) := \langle F \rangle : h_F^\infty = \{f \in \Bbbk[\mathbf{x}] \mid \exists k \in \mathbb{N} \text{ s.t. } h_F^k f \in \langle F \rangle\}.$$

Definition 2.37.
A triangular set $F \subset \Bbbk[\mathbf{x}]$ is a **regular chain** if either $F = \varnothing$ or $\text{ires}(h_F, F) \neq 0$. This is equivalent to saying that h_F is **regular** modulo $\text{sat}(F)$ (meaning that h_F is neither zero modulo $\text{sat}(F)$, nor a zero divisor modulo $\text{sat}(F)$).

A **regular system** is a pair $[F, h]$ such that F is a regular chain and $\text{ires}(h, F) \neq 0$. The **zero set** of $[F, h]$ is $Z(F, h)$ (recall this equals $\mathbf{W}(F) \setminus \mathbf{V}(h)$ and $\mathbf{W}(F) = \mathbf{V}(F) \setminus \mathbf{V}(h_F)$).

A **triangular decomposition** of a zero-dimensional variety produces a sequence of regular systems such that their zero sets decompose the zero system of the original system.

Triangular decompositions have many desirable properties due to that fact the initials of the polynomials in a regular chain behave nicely. For example, the variety of a regular chain is **equiprojectable**: all fibers of the projection map on the variety have the same cardinality [DMS+04].

2.5.2 Recursive Regular Chains CAD (RC-Rec-CAD)

The new algorithm for CAD introduced in [CMXY09] makes use of triangular decompositions to tackle CAD. Whereas the original algorithm was rooted purely in $\mathbb{R}^n$, the

new algorithm first decomposes $\mathbb{C}^n$. The idea of a cylindrical decomposition of $\mathbb{K}^n$ (for which we will think of $\mathbb{C}^n$) is needed, analogous to Definitions 2.11 and 2.12.

Definition 2.38 ([CMXY09])**.**
A **cylindrical decomposition**, $\mathcal{D}$, of $\mathbb{K}^n$ is defined recursively:

- If $n = 1$ then $\mathcal{D} = \{D_1, \ldots, D_{m+1}\}$ where either:
  - $m = 0$ and $D_1 = \mathbb{K}$; or
  - $m > 0$ and there exists m non-constant, squarefree, co-prime $f_1, \ldots, f_m \in \Bbbk[\mathbf{x}]$ such that for $1 \leq j \leq m$:

$$D_j = \{z_1 \in \mathbb{K} \mid f_1(z_1) = 0\} \quad \text{and} \quad D_{m+1} = \{z_1 \in \mathbb{K} \mid \prod_{j=1}^{m} f_j(z_1) \neq 0\}.$$

- If $n > 1$, let $\mathcal{D}' = \{D_1, \ldots, D_s\}$ be a cylindrical decomposition of $\mathbb{K}^{n-1}$. For each D_i let $\{f_{i,1}, \ldots, f_{i,m_i}\} \subseteq \Bbbk[\mathbf{x}]$ be a set of polynomials that **separates** above D_i (for all $\alpha \in D_i$, $(\text{init}(f_{i,j}))_\alpha \neq 0$ and $\{(f_{i,j})_\alpha\}_{j=1}^{m_i}$ are co-prime).
  - If $m_i = 0$ then $D_{i,1} = D_i \times \mathbb{K}$.
  - If $m_i > 0$ then for $1 \leq j \leq m_i$:

$$D_{i,j} = \{(\alpha, z_n) \in \mathbb{K}^n \mid \alpha \in D_i, f_{i,j}(\alpha, z_n) = 0\} \quad \text{and}$$
$$D_{i,m_i+1} = \{(\alpha, z_n) \in \mathbb{K}^n \mid \alpha \in D_i, \prod_{j=1}^{m_i} f_{i,j}(\alpha, z_n) \neq 0\}.$$

  The collection $\mathcal{D} = \{D_{i,j} \mid 1 \leq i \leq r, 1 \leq j \leq r_i\}$ is then a cylindrical decomposition of $\mathbb{K}^n$.

The concept of sign-invariance (Definition 2.16) is generalised to $\mathbb{C}^n$:

Definition 2.39 ([CMXY09])**.**
Let $f \in \mathbb{Q}[\mathbf{x}]$ and R a region of $\mathbb{C}^n$. We say that f is **invariant** on R if either:

1. $f(\alpha) = 0$ for all $\alpha \in R$; or
2. $f(\alpha) \neq 0$ for all $\alpha \in R$.

Let $F \subset \mathbb{Q}[\mathbf{x}]$. Then R is F**-invariant** if every polynomial in F is invariant on R. A decomposition of $\mathbb{C}^n$ is F**-invariant** if every cell is F-invariant.

The algorithm for a set of polynomials $F \subset \mathbb{Q}[\mathbf{x}]$ then consists of three main steps:

1. `InitialPartition`: Decomposes $\mathbb{C}^n$ into **constructible sets** (a finite combination of algebraic varieties by set union and difference) that are F-invariant using triangular decomposition techniques.

2. `MakeCylindrical`: Transforms the constructible sets into an F-invariant cylindrical decomposition of $\mathbb{C}^n$.

3. `MakeSemiAlgebraic`: Transforms the cylindrical decomposition of $\mathbb{C}^n$ into an F-invariant cylindrical algebraic decomposition of $\mathbb{R}^n$.

Whilst the initial implementation means that this algorithm is often less time-efficient than implementations of Collins' algorithm, it can often produce CADs with much fewer cells. Due to many of the algorithms being recursive in nature, we refer to this algorithm as the **recursive regular chains algorithm**, or **RC-Rec-CAD**.

2.5.3 Incremental Regular Chains CAD (RC-Inc-CAD)

Recently [CM12], a new algorithm has been published improving on the one described in Section 2.5. Their approach is still to create an F-invariant cylindrical decomposition of $\mathbb{C}^n$ and apply `MakeSemiAlgebraic` to produce an F-invariant CAD of $\mathbb{R}^n$. Their method of creating the cylindrical decomposition of $\mathbb{C}^n$ differs significantly however, utilising an incremental approach.

Rather than thinking in terms of a decomposition, they construct a complex cylindrical tree.

Definition 2.40 ([CM12])**.**
We define the **complex cylindrical tree** (**CCT**) for a cylindrical decomposition of $\mathbb{C}^n$ by induction on n. For $n = 1$, let $\mathcal{D} = \{D_1, \ldots, D_{r+1}\}$ be a cylindrical decomposition. The tree associated with $\mathcal{D}$ is a rooted tree whose nodes, other than the root, are $D_1, \ldots, D_{r+1}$, which all are leaves and children of the root.

Now let $n > 1$, $\mathcal{D} = \{D_{i,j} \mid 1 \leq i \leq s, 1 \leq j \leq r_i+1\}$ be the cylindrical decomposition of $\mathbb{C}^n$, over the induced cylindrical decomposition $\mathcal{D}' = \{D'_1, \ldots, D'_s\}$ of $\mathbb{C}^{n-1}$ (where $\{D_{i,j} \mid 1 \leq j \leq r_i\}$ are the cells in the cylinder over D'_i). If T' is the tree associated with $\mathcal{D}'$ then the tree T associated with $\mathcal{D}$ is defined as follows. For each $1 \leq i \leq s$ the set D'_i is a leaf in T' which has all $D_{i,j}$'s for children in T; thus the $D_{i,j}$'s are the leaves of T.

The complex tree can be thought as a mathematical realisation of the `piecewise` output of CAD in Maple [CDM+09]. Starting with the trivial cylindrical tree (the tree

of depth n where each condition is simply "$\forall x_j$") they 'refine' along each path from the root with each of the polynomials in F. This refinement consists of taking the greatest common divisors of the irreducible factors of the current polynomial with the conditions.

With this new method, the algorithm can make use of equational constraints and certain partial CAD techniques (using the quantifier structure of the problem), which were incompatible with the recursive method described in Section 2.5. With these additions the new algorithm seems to outstrip all other algorithms on most examples [CM12]. Further, this method can be used for quantifier elimination, which has been implemented and investigated for future publication [CMM14].

As this algorithm incrementally refines the complex cylindrical tree before constructing the CAD, we refer to this algorithm as the **incremental regular chains algorithm**, or **RC-Inc-CAD**.

2.6 Complexity of Cylindrical Algebraic Decomposition

Cylindrical algebraic decomposition improved on the complexity of Tarski's original decision method [Tar51], which had non-elementary complexity. However, constructing a cylindrical algebraic decomposition is still a difficult procedure, as shown by the complexity results detailed in this section.

2.6.1 Formal Complexity of CAD and QE

In [DH88] the authors prove that quantifier elimination and CAD are both inherently doubly exponential in the number of variables, n.

This is done by converting the complex equation:

$$x_1^{2^{2^{j+1}}} = x_2$$

into a quantified real formula ϕ_j in variables $x_{1R}, x_{1I}, x_{2R}, x_{2I}$ where $x_j = x_{jR} + ix_{jI}$. Then setting $x_2 = 1$ gives the $2^{2^{j+1}}$ roots of unity.

Considering the decomposition of $\mathbb{R}^{6j+2}$ induced by ϕ_j, it must contain at least $2^{2^{j+1}}$ 0-dimensional cells. Therefore, in terms of the number of variables, n, we obtain a lower bound in complexity of

$$2^{2^{(n-2)/6}}. \tag{2.2}$$

This can be improved slightly by perturbing ϕ_j to get

$$2^{2^{(n-2)/5}}. \tag{2.3}$$

The best upper bounds of the time had an exponent of $n + \log n + 5$ leaving a large working range.

In [BD07] the authors improve on this result in a variety of ways. Their bound is tighter, requires only linear polynomials and does not assume a dense representation of polynomials. They also prove results about variable ordering which will be discussed in Section 2.6.3.

Their construction starts with the piecewise function:

$$f_0(x) = \begin{cases} 2x & \text{for } x \leq \frac{1}{2} \\ 2 - 2x & \text{for } x > \frac{1}{2} \end{cases} ;$$

and $f_0^{(k)}$ is the k-fold composition of f_0. It is easy to define a quantified formula $\Phi_n(x_n, 1/2)$ which defines the midpoints of the segments of the graph of $f_0^{(k)}$ on $[0, 1]$. The bound the authors achieve is

$$2^{2^{(n-1)/3}}. \tag{2.4}$$

2.6.2 Complexity of CAD Algorithms

The complexity results in [DH88] and [BD07] are lower bounds for the complexity of certain CADs. This does not inform us about the complexity of specific algorithms. We summarise the known results here.

Collins' Algorithm

In [Col75], after introducing the original CAD algorithm Collins gives a detailed complexity analysis of its execution. For an input of m polynomials with degree d in n variables with maximum norm length of coefficients l the complexity is:

$$O\left((2d)^{2^{2n+8}} m^{2^{n+6}} l^3\right). \tag{2.5}$$

Collins notes that the exponents in (2.5) can likely be reduced by using more efficient subalgorithms (stating the exponent of l reduces from 3 to $2 + \epsilon$ for any $\epsilon > 0$) and by a tighter analysis of the CAD algorithm (stating that the initial exponent of $2n + 8$ could reduce to $2n + 4$). The analysis will be given in more detail in Section 4.5 in the context of analysing a new algorithm.

McCallum's CADMD Algorithm

In [McC93] the author introduces an algorithm to construct only the full dimensional cells of a CAD (discussed in Section 2.4.5). The production of fewer cells and avoidance of computations with algebraic numbers (all sample points are in $\mathbb{Q}^n$) offers large savings and McCallum gives a complexity analysis producing:

$$O\left((2d)^{3^{n+4}} m^{2^{n+4}} l^3\right). \tag{2.6}$$

The exponents in (2.6) are smaller than (2.5) (as $3^{n+4} < 2^{2n+8} = 4^{n+4}$). This analysis will be revisited in detail in Section 4.5 when analysing a new algorithm.

Remark 2.5.
Whilst the lower bounds of (2.2), (2.3), (2.4) and the upper bounds of (2.5), (2.6) are all doubly exponential in n, they do *not* imply that CAD is $2^{2^{\Theta(n)}}$. There is a large range of permissible complexities and a small difference in the double exponent (such as between (2.5) and (2.6)) can offer huge savings in an implementation.

Also note that for a fixed n the complexities are polynomial in d, m and l. As the exponents of d and m depend exponentially on n, any reduction in the value of the linear terms in n will have a significant effect.

2.6.3 Variable Ordering for CAD

For a given set of polynomials the choice of variable ordering can make a significant difference to the complexity of the CAD produced. This was demonstrated in [BD07] where a single polynomial was given in $3n + 3$ variables that produced 3 cells for a particular ordering, but 2^{2^n} cells with a different projection ordering. Note that there is not always a "good" variable ordering; the same paper produced a set of $3n^2$ polynomials in $3n + 1$ variables that produces a CAD with at least 2^{2^n} cells with any of the $(3n + 1)!$ projection orders.

Identifying a computationally easy way to identify an optimal variable ordering for a given problem is of great importance. For quantifier elimination problems the choice of variable ordering is restricted to admissible orderings.

Definition 2.41.
Let Φ be a quantifier elimination problem. Let the quantifiers in Φ be

$$(Q_k x_k)(Q_{k+1} x_{k+1}) \cdots (Q_n x_n).$$

We can group together adjacent quantifiers of the same type (as $\forall x \forall y \leftrightarrow \forall y \forall x$ and $\exists x \exists y \leftrightarrow \exists y \exists x$) to give the **block representation** of Φ as:

$$(\hat{Q}_1 B_1) \cdots (\hat{Q}_r B_r) \varphi$$

where $\hat{Q}_i \neq \hat{Q}_{i+1}$ for $i = 1, \ldots, r-1$ and the B_i are a partition of $\{x_k, \ldots, x_n\}$ respecting their order. An **admissible ordering** for Φ is any which projects the variables of B_r first, followed by B_{r-1}, and so forth until B_1, followed by any ordering of $x_1, \ldots, x_{k-1}$.

In [DSS04], the authors systematically tested a collection of metrics to find the one which best correlates with CAD complexity. The most appropriate metric was found to be the sum of total degrees, `sotd`.

Definition 2.42 ([DSS04])**.**
For a set of polynomials $F \subset \mathbb{Q}[\mathbf{x}]$ and variable ordering $\hat{\mathbf{x}}$, the **sum of total degrees**, $\texttt{sotd}(F, \hat{\mathbf{x}})$, is defined to be:

$$\texttt{sotd}(F, \hat{\mathbf{x}}) = \sum_{i=1}^{n} \sum_{f \in F_i} \sigma(f)$$

where $F_1, \ldots, F_n$ are the projection sets of F with respect to $\hat{\mathbf{x}}$ and $\sigma(f)$ sums the total degrees of each monomial in f.

In [Bro04] a simple heuristic for deciding variable ordering was given.

Definition 2.43 ([Bro04])**.**
The **Brown heuristic** assigns the order of variables to be eliminated according to the following conditions (breaking ties with successive conditions):

1. Descending order by degree of variable;
2. Descending order by highest total-degree term in which the variable appears;
3. Descending order by the number of terms containing the variable.

This is computationally simple, and performs remarkably well. However, Phisanbut noticed ([Phi11]) that this heuristic does not distinguish between coupled variables (real variables arising from the same complex variable) in Branch Cut Analysis (Section 2.8.1).

These heuristics will be revisited with respect to variable ordering in Chapter 5, as well as in Chapters 3, 6, and 7.

2.7 Adjacency in Cylindrical Algebraic Decomposition

Given a CAD, it is often important to know the adjacency of cells. Although it will not be a focus of the research in this thesis, we give the appropriate definitions, as it has important implications on CAD algorithms and properties of CADs that enable easier adjacency computations. Further details are given in Appendix A.

We have two alternative definitions for adjacency in a CAD, which we will refer to as **(A1)** and **(A2)**.

Definition 2.44.
Given two disjoint cells D_1, D_2 of $\mathbb{R}^n$ we say they are **adjacent** if either:

(A1) their union, $D_1 \cup D_2$, is connected.

(A2) the cell of smaller dimension is entirely contained in the closure of the larger-dimensional cell.

If D_1, D_2 are adjacent regions, we call the set $\{D_1, D_2\}$ an **adjacency**. If unclear, we can specify an **(A1)**-adjacency or **(A2)**-adjacency.

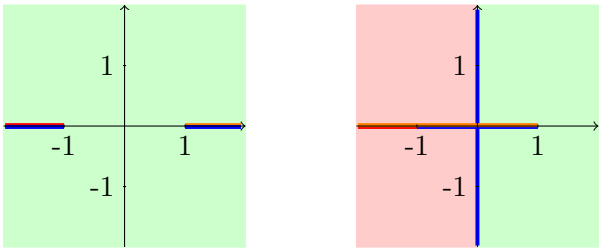
If $\{D_1, D_2\}$ is an **(A2)**-adjacency and D_2 is the cell of smaller dimension, we say D_2 is a **face** of D_1.

Whilst **(A2)** implies **(A1)**, the converse is not true and so **(A1)** and **(A2)** are not equivalent definitions. Details on algorithms to compute adjacencies of a CAD and to use such adjacencies to improve construction are described in Appendix A.

2.8 Applications of Cylindrical Algebraic Decomposition

The use of CAD for quantifier elimination opens up many applications. Quantifier elimination is important for many areas of mathematics, science and engineering.

There are a variety of applications for cylindrical algebraic decompositions, along with quantifier elimination. Five applications we briefly discuss are the analysis of branch cuts in complex identities, robot motion planning, automated theorem proving, formal verification of dynamical systems, and an automated examination question answering system.



(a) Identity (2.7). (b) Identity (2.8).

Figure 2.2: Branch Cut geometry for identities involving square roots.

2.8.1 Branch Cut Analysis

Consider the problem of deciding the validity of the two following identities over $\mathbb{C}$:

$$\sqrt{1-z}\sqrt{1+z} \stackrel{?}{=} \sqrt{1-z^2}; \tag{2.7}$$

$$\sqrt{z-1}\sqrt{z+1} \stackrel{?}{=} \sqrt{z^2-1}. \tag{2.8}$$

In [PBD11] (and further discussed in [Phi11]) the authors stress how the geometry of the branch cuts involved in an identity are key to discovering its validity. If we look at Figure 2.2 we can see:

- The branch cuts of (2.7) do not divide the complex plane and the identity is true over the whole plane.
- The branch cuts of (2.8) divide the complex plane into three regions and the identity is false on two of these regions.

Note that this is typical but not universal behaviour: examples exist where the complex plane is split but an identity holds everywhere, or where the plane is not split but the identity fails on the branch cuts themselves.

An automatic procedure for deciding validity of such problem can be created using CAD. For a given complex identity the steps of Algorithm 2.5 are carried out [BPB05, Phi11].

Branch cut verification will be revisited in Chapter 3 as an application particularly suited to the advances described in that chapter.

Algorithm 2.5: `Verify`: Complex identity verification (with CAD) algorithm.

1 Find a possible simplification;
2 Check 'algebraically' it is correct (e.g. using `simplify(..,symbolic)` in MAPLE);
3 Check correctness for branch cuts:

i. Determine all branch cuts;

ii. Represent them as semi-algebraic equations in $\Re(z)$ and $\Im(z)$;

iii. Generate a CAD of $\mathbb{C}^n = \mathbb{R}^{2n}$ according to the branch cuts;

iv. Evaluate at the sample point of each cell: the simplification is either identically true or *generically* false on cell;

2.8.2 Robot Motion Planning

Problem 2.2 (Piano Mover's Problem)**.**
Given an object in a space filled with other objects, is there a path from one specified point to another without any objects colliding?

In [SS83b], the authors described a way to solve Problem 2.2 using CAD. The authors describe a method of rewriting objects as semi-algebraic sets and translating these into conditions to ensure safe passage of the robot. Inputting into a CAD algorithm would then provide cells where the robot can safely traverse to. However, in [Dav86] a simple example is considered (a 3m ladder in a right-angled corridor of 1m width) and shown to be too complex for CAD technology. Even with current algorithms and computing power, this example still proves too complex without geometric reasoning.

More recently, [Lee11], CAD has also been used as a subprocedure of a spatial-awareness algorithm for robots using artificial intelligence techniques.

The Piano Mover's Problem will be revisited in Chapter 6, where a reformulation of the problem allows for a cylindrical algebraic decomposition to be created in a reasonable amount of time.

2.8.3 Automated Theorem Proving

Decision methods for the first order theory of the reals have been used in automatic theorem proving in a variety of ways. In [DSW98] the authors translate geometrical theorems into quantifier elimination problems. A simple example is the theorem that

two lines intersect at one and only one point, which translates to:

$$\exists x \forall y (mx + b = 0 \wedge (y = x \vee my + b \neq 0)). \tag{2.9}$$

Although they state, quite correctly, that QEPCAD is insufficient for most non-trivial examples on its own, they do use it as an intermediary tool. This is often to prove that their reformulation is equivalent to the problem being queried.

QEPCAD is also used within the automatic theorem tool METITARKSI which proves results regarding elementary functions by restating them in terms of polynomial bounds. This was first introduced in [AP08] and later extended in:[AP09, PPdM12]. There has been much work done on optimising this code and it is often the state-of-the-art.

2.8.4 Formal Verification of Dynamical Systems

The work in [ST11] (building on work such as [Jir97, Ioa97]) describes formally verifying and synthesising (continuous and switched) dynamical systems. By reducing a dynamical system's behaviour to a first-order formula over the reals, quantifier elimination can be used to investigate its behaviour. Four case studies are given: avoiding crashes with adaptive cruise control in cars; applying force to a robot to maintain a certain position; ensuring stability with adaptive flight control; and maintaining an inverted pendulum in its unstable equilibrium.

Reducing behaviour of a system to a quantified formula the authors then follow a three step process: eliminating all variables that are allowed (due to the degree bounds) by virtual substitution (described in Section 2.9.2); using SLFQ to apply black-box preconditioning (described in Section 2.4.6) to the resulting formula; constructing a CAD for the (possibly still quantified) preconditioned formula and to provide an equivalent description of the behaviour of the system. They also note that the quantifier-free formulae generated from CAD-based QE algorithms are very understandable: *"it is well-known that elimination results of CAD, in contrast to most other QE methods, are very concise, nonredundant, and intuitively interpretable"* ([ST11]).

2.8.5 Automated Examination Question Answering System

The Todai Robot Project[5] aims to create an automated system to pass the Tokyo University entrance exam by 2021 [AMIA14, MIAA14]. The exam consists of seven subject areas, including mathematics, and the automated system must interpret each exam ques-

[5] `http://21robot.org/`

tion, discover a solution (using methods depending on the subject area), and construct an answer.

Approximately 47% of the mathematics questions on the entrance exams can be expressed in the theory of real closed fields [MIAA14, Table 1], and can be solved by quantifier elimination. A hybrid system is used, applying virtual substitution and Sturm-Habicht sequences, where appropriate, before appealing to CAD to solve these questions. As the automated translation from the exam script to a quantified formula often produces overly-complicated input with many variables, preconditioning of the input is essential (including techniques discussed in [WBD12] and Chapter 6).

2.9 Alternatives to Cylindrical Algebraic Decomposition

CAD is not the only alternative to Tarski's original decision algorithm for the first order theory of the reals, nor the only algorithm for analysing semi-algebraic sets. Although CAD vastly improves on the theoretical complexity of Tarski's algorithm, it is possible to improve it further. This section is not intended to be an in-depth discussion of these algorithms but an overview to offer a frame of reference to CAD. Nor is this section intended to particularly justify the study and use of CAD or alternative algorithms: there are situations where particular algorithms are more well-suited, and the study of CAD in this thesis is intended purely to improve CAD's efficiency.

2.9.1 Singly-exponential Algorithms

The first decision algorithm for the existential theory of the reals that had singly exponential complexity was presented by Grigor'ev and Vorobjov in [Gri88, GV88]. This was improved upon in a series of papers by a range of authors, culminating in a trio of papers by Renegar [Ren92a, Ren92b, Ren92c]. We will try to outline the basic ideas behind these results as discussed and aggregated in [BPR06].

A problem is translated into an alternative question: for a set of polynomials, $F \subset \mathbb{R}[\mathbf{x}]$, find the corresponding set of all **realisable sign conditions**, $\text{Sign}(F) \subseteq \{-1, 0, 1\}^F$. This is sufficient to decide existence of a solution to a Tarski formula.

The polynomials are then translated into **strong l-general position** with respect to a polynomial $q \in \mathbb{R}[\mathbf{x}]$. First the set F needs to be partitioned into subsets $\{F_i\}_{i=1}^s$ such that, for each i, no two elements of F_i have a common zero in $\mathbb{R}^n$. Further, no $l+1$ polynomials belonging to different F_i can have a zero in common with q in $\mathbb{R}^n$. Moreover, any l polynomials belonging to different F_i can have at most a finite number

Algorithm	Theoretical Complexity
Collins CAD	$(md)^{2^{O(n)}}l^3$
Grigor'ev/Vorobjov	$(md)^{n^2}l$
Renegar	$(md)^{O(n)}l(\log l)(\log\log l)$

Table 2.1: Theoretical complexities of decision algorithms.

of zeros in common with q in $\mathbb{R}^n$ (if this does not hold then the general position is not considered strong). Often q is taken to be the zero polynomial, whence the polynomials are simply said to be in **strong l-general position**.

By considering the introduction of two infinitesimals, a strong relationship is shown between the sign conditions of a set of polynomials and the weak sign conditions of their translation to general position. These are much easier to work with, although an additional (non-trivial) step is needed to remove these infinitesimals from the produced sample points.

This results in an algorithm that can decide the existence of a solution to a formula involving m polynomials in n variables, each of degree at most d with complexity $m^{n+1}d^{O(n)}$.

Practical Efficiency Comparison of Critical Point Methods with CAD

In [Hon91] the author compared three decision algorithms for the existential theory of the reals: CAD, the general Grigor'ev/Vorobjov method, and Renegar's improvement to the Grigor'ev/Vorobjov algorithm. Considering their theoretical complexities it seems obvious that Grigor'ev/Vorobjov and Renegar are the more efficient algorithms. Table 2.1 shows the theoretical complexities: n is the number of variables; m the number of polynomials; d the maximum total degree; and l the maximum bit length for coefficients.

Obviously theoretical complexity can betray practical behaviour when algorithms are implemented. Whilst CAD had been fully implemented, the general Grigor'ev/Vorobjov and Renegar algorithms had not and Hong considered a theoretical implementation of these.

Hong considered the simple case where $n = m = d = l = 2$: at most two polynomials in two variables with maximum total degree two and coefficients in the set $\{-1, 0, 1\}$. There are $3^{12} = 531,441$ pairs of polynomials satisfying $n = m = d = l = 2$ and Hong tested each of these with an implementation of CAD (that would later form the basis of QEPCAD) and found they all completed within 10-200 milliseconds.

Hong then worked with the equation:

$$(\exists x_1)(\exists x_2)[x_1^2 + x_2^2 < 1 \wedge x_1 x_2 > 1], \tag{2.10}$$

solving (2.10) with each of the three algorithms.

As expected by the practical results above, it is rather simple to work through (2.10) with the CAD algorithm and this can be easily done by hand. However, Hong estimates that solving (2.10) with the Grigor'ev/Vorobjov algorithm or Renegar's algorithm would take well over a million years.

From these results it would seem clear that if the aim is for practical quantifier elimination, CAD is the optimal algorithm. However, there has been substantial progress in both CAD and critical point algorithms since then and, in particular, there are special cases of the critical point algorithm that can be highly efficient. These are discussed in the following section.

Special Cases of Critical Point Algorithms

In [HRS93] the authors also restrict themselves to the existential theory of the reals and respond to the discussion in [Hon91] by proposing the idea: *" It is possible to implement efficiently slight variants of single exponential methods well adapted to important particular cases of the decision problem"* ([HRS93]).

They explain that the key idea of the critical points algorithms is to work directly on the geometrical object. Deciding a problem in the existential theory of the reals equates to deciding if a given semi-algebraic set in $\mathbb{R}^n$ is non-empty, and the authors pointed out this does not require much of the information encoded in the projection set for CAD. They describe how to deal with a smooth bounded regular hypersurface, where the critical points algorithms reduce to a straightforward Gröbner basis computation (and so is very efficient). They then list a sample of other special cases and point out that it is possible to start the computations assuming the geometric situation is good and only appeal to the more sophisticated algorithms if necessary.

There have been many advances since the discussions in [Hon91, HRS93] and [Vor03, BPR06] give detailed discussions, including complexity analysis of the algorithms. Certain critical point algorithms have been implemented in the RAGLib package[6] for Maple.

[6] `http://www-salsa.lip6.fr/~safey/RAGLib/`

2.9.2 Virtual Substitution

Amongst the alternative quantifier elimination methods that are not based on critical points, the **virtual substitution** method first introduced in [Wei97] is of particular note. Through a sequence of smart substitutions (such as for the solution to a quadratic or perturbing a variable by an infinitesimal) variables can be tested for various cases and eliminated by combining these cases. This process is very efficient but it is restricted by the degree in the candidate variable, which must be linear or quadratic, and this restriction can be affected by successive eliminations (increasing the degrees of other variables). Further, it often produces a very large output formula, although there have since been improvements (such as [Bro05a] which also provides a survey of the subject).

The virtual substitution method of quantifier elimination is implemented in the REDLOG package[7] within the REDUCE computer algebra system. Virtual substitution is also one of the techniques employed in SYNRAC[8].

2.10 Formalisation of Cylindrical Algebraic Decomposition

There has been work [Mah07, MC12] to formalise the CAD algorithm in the proof assistant COQ. Using the SSREFLECT library [GM10], Mahboubi has implemented the CAD algorithm within COQ but has not yet proven it is correct. A quantifier elimination procedure has been implemented and verified within COQ [CM10, MC12], which combines ideas from Tarski's algorithm and CAD. If CAD could be formalised within COQ then it may lead to a greater understanding of the algorithm and properties. A comprehensive description of the current progress is given in [Coh13].

2.11 Implementations of Cylindrical Algebraic Decomposition

There are a range of implementations of CAD. One of the most well-used is QEPCAD (specifically QEPCAD-B 1.69 [Bro03]) which is written in `C` using the `Saclib` library and implements Collins' algorithm (Section 2.3) with suitable extensions (Section 2.4).

Within commercial computer algebra software there are implementations in the `RegularChains` library of MAPLE 16+ (which is based on the alternative algorithm described in Section 2.5) and MATHEMATICA (which is based on Collins' algorithm of Sec-

[7] `www.redlog.eu/`

[8] `http://jp.fujitsu.com/group/labs/techinfo/freeware/synrac/`

tion 2.3 but with further extensions by Strzeboński as described in [Str06, Str11, Str12]). The incremental algorithm for Cylindrical Decomposition described in Section 2.5.3 is implemented over the `RegularChains` library and will be freely available[9].

MATHEMATICA uses heuristics and meta-algorithms to precondition input and often uses techniques such as Gröbner Bases when more appropriate than CAD. The CADs are often not cylindrical in the Collins' sense: they are cylindrical with respect to themselves, not necessarily the overall decomposition. To this extent it is often hard to compare Mathematica with other implementations of CAD.

There are a small handful of other implementations, including REDLOG[10] (within REDUCE, using virtual substitution [Wei97] and generic partial CAD [SS03]), the MAPLE package SYNRAC[11] (using validated numerics to combine a symbolic and numeric approach, as well as some virtual substitution techniques), and the CADPUB package in AXIOM[12] (using ideas related to the real closure of fields [Rio92]).

To assist in investigation of features of CAD we require a fully transparent implementation of the algorithms involved. To this end, an implementation of CAD by projection was created by the University of Bath computer algebra group and is documented in [Eng13a, Eng13b]. This package, PROJECTIONCAD, features both Collins' and McCallum's projection methods along with many algorithms related to CAD, using sub-procedures from the `RegularChains` package [EWBD14]. The `ProjectionCAD` package also includes much of the work featured in this thesis, notably implementations of key algorithms from Chapters 3 and 4 (the latter by the author of this thesis). The implementation of `ProjectionCAD` is discussed further in Appendix C.

2.12 Solotareff-3

"**Solotareff-3**" is an often-quoted problem within CAD experimentation, but is stated in various ways. An interesting example of an application of CAD, we introduce it as a motivating example in Section 1.3 and will revisit this problem in Sections 3.10, 4.8, 5.5, 6.5 and 7.4 to discuss how the various advances in CAD theory can be used to improve the efficiency solving this problem. Whilst CAD is not the only way to solve the Solotareff problems, it proves a useful example to consider for each topic discussed in this thesis.

[9] `www.regularchains.org`
[10] `www.redlog.eu/`
[11] `http://jp.fujitsu.com/group/labs/techinfo/freeware/synrac/`
[12] `http://rioboo.free.fr/CadPub/`

Problem 2.3 (The Solotareff Problem)**.**
Find the closest approximation, with respect to the uniform norm [13] on $[-1, 1]$, of a polynomial of degree n by a polynomial of degree $n-2$ or less.

Solotareff first posed this question in 1933 and it is clearly equivalent to approximating the binomial $x^n + rx^{n-1}$ by a polynomial of degree $n-2$.

2.12.1 Description of Solotareff-3

We will consider the case when $n = 3$. Let S and P be the following polynomials:

$$S := x^3 + rx^2, \qquad P := ax + b. \tag{2.11}$$

Solotareff-3 involves finding algebraic expressions, in terms of r, for a and b such that P most closely approximates S on $[-1, 1]$.

We can use the definition of uniform norm to formulate the problem as follows:

$$(\forall\ d)(\forall\ e)(\forall\ x)(\exists\ y)\Big[[-1 \le x \le 1] \Rightarrow [-1 \le y \le 1] \wedge \\ [((x^4 + rx^3) - (ax + b))^2 \le ((y^4 + ry^3 - dy + e))^2]\Big]. \tag{2.12}$$

Processing this with a CAD algorithm, and performing quantifier elimination would produce a decomposition of $\mathbb{R}^3$ with expressions of a, b for all values of r. However, this is too complex a problem for CAD to be of use.

We use an reformulation of Achieser [Ach56] restricted to the case $r = -1$:

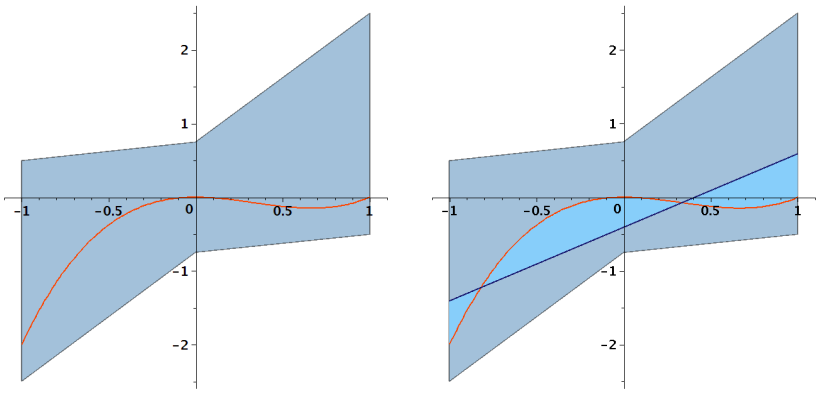
$$(\exists\ u)(\exists v)\Big[[3v^2 - 2v - a = 0]\ \wedge\ [v^3 - v^2 - av - 2b + a - 2 = 0] \\ \wedge\ [3u^2 - 2u - a = 0]\ \wedge\ [u^3 - u^2 - au - a + 2 = 0]\ \wedge\ [1 \le 4a]\ \wedge\ [4a \le 7] \\ \wedge\ [-3 \le 4b]\ \wedge\ [4b \le 3]\ \wedge\ [-1 \le v]\ \wedge\ [v \le 0]\ \wedge\ [0 \le u]\ \wedge\ [u \le 1]\Big], \tag{2.13}$$

which is quoted as an example in [BH91]. The problem is shown in Figure 2.3a: we are finding the line within the shaded region that closest approximates the given cubic.

We will concentrate on (2.13) throughout this thesis, considering how we can construct a CAD for this formula more efficiently.

CAD has also been used to solve the Solotareff-4 problem [Col97]. By considering the Zariski closure (and using an alternative to CAD to analyse the semi-algebraic set) Solotareff-n has been algorithmically solved up to $n = 12$ [Laz06].

[13] The **uniform norm** on a set S, $\|f\|_{\infty,S}$, is defined to be $\sup\{|f(x)| \mid x \in S\}$.



(a) Solotareff-3 problem. (b) Solution to Solotareff-3.

Figure 2.3: Solotareff-3 from [BH91]: identify the line within the given region that best approximates the cubic with respect to the uniform norm on $[-1, 1]$.

2.12.2 Experimental Results for Solotareff-3 with Current Technology

We construct a CAD for the Solotareff-3 problem described in (2.13) with the current technology. We are partly restricted in variable ordering due to the quantifier structure, and so consider the two orderings $a \prec b \prec v \prec u$ and $b \prec a \prec v \prec u$. The results are summarised in Tables 2.2 and 2.3.

Projection and Lifting CAD in `ProjectionCAD`

We can use the implementations of projection and lifting CAD in `ProjectionCAD` to construct a CAD with respect to Collins' projection operator (Definition 2.22) or McCallum's projection operator (Definition 2.24). With the first variable ordering, both Collins' and McCallum's operators give $54,047$ cells in around four minutes. The second variable ordering proves more difficult, producing $161,317$ cells with Collins' operator and $154,527$ cell with McCallum's operator, taking around fifteen minutes.

We can utilise two of the equational constraints (f_3 and f_4) from (2.13): those equational constraints containing the main variable u. Doing so produces about a third of the cells: $20,539$ and $22,109$ cells for the first variable ordering (taking between one and two minutes); $48,475$ and $63,583$ for the second variable ordering (taking between three and six minutes).

Technique	Cells	Time	Section	Page
PL-CAD (Col)	54037	255.304	2.3	30
PL-CAD (McC)	54037	266.334	2.3	30
EC-CAD (f_3)	20593	65.856	2.4.4	40
EC-CAD (f_4)	22109	102.781	2.4.4	40
QEPCAD (full-cad no $\exists$)	54037	5.701	2.11	58
QEPCAD (no $\exists$)	1015	4.807	2.11	58
QEPCAD (full-cad)	349	4.782	2.11	58
QEPCAD	153	4.659	2.11	58
RC-Rec-CAD	54037	327.421	2.5	43
RC-Inc-CAD	29	0.155	2.5.3	46
RC-Inc-ECCAD	29	0.149	2.5.3	46

Table 2.2: The Solotareff-3 problem with current technology — variable order $a \prec b \prec v \prec u$.

Partial CAD in QEPCAD

We can use QEPCAD to eliminate the variables in (2.13) and so solve the Solotareff problem in this case. Using the ordering $a \prec b \prec v \prec u$ we get the following equivalent quantifier-free formula:

$$a - 1 = 0 \wedge 4b + 3 > 0 \wedge 27b^2 - 18ab + 56b - a^3 + 2a^2 - 19a + 29 = 0,$$

which gives the solution: $a = 1, b = -\frac{11}{27}$. Using the variable ordering $b \prec a \prec v \prec u$ we get the answer directly: $27b + 11 = 0 \wedge a - 1 = 0$.

Therefore we have found that the closest linear approximation to the polynomial $x^3 - x^2$ under the uniform norm on the interval $[-1, 1]$ is $x - \frac{11}{27}$. This completely solves the Solotareff-3 problem when $r = -1$, and is demonstrated in Figure 2.3b.

By using the `d-stat` and `d-fpc-stat` commands we can get information regarding the CADs constructed to solve this problem. Allowing QEPCAD to fully use its partial CAD and equational constraints techniques results in a partial CAD of $\mathbb{R}^2$ containing 153 cells for the first variable ordering (constructing $1,100$ cells in the process of solving the problem) and 375 cells for the second variable ordering (constructing $2,228$ cells in the process of solving the problem). Specifying `full-cad` limits certain partial techniques, producing 349 cells ($1,314$ total cells constructed) and $1,063$ cells ($2,950$ total cells constructed) in the two-dimensional CAD. We can also remove the existential quantifiers, to build a partial CAD of $\mathbb{R}^4$ with $1,015$ cells ($1,100$ total cells constructed) and $2,065$ cells ($2,228$ total cells constructed). Removing the quantifiers and specifying

Technique	Cells	Time	Section	Page
PL-CAD (Col)	161317	916.105	2.3	30
PL-CAD (McC)	154527	857.357	2.3	30
EC-CAD (f_3)	48475	175.139	2.4.4	40
EC-CAD (f_4)	63583	324.663	2.4.4	40
QEPCAD (full-cad no $\exists$)	154527	8.249	2.11	58
QEPCAD (no $\exists$)	2065	4.785	2.11	58
QEPCAD (full-cad)	1063	4.832	2.11	58
QEPCAD	375	4.687	2.11	58
RC-Rec-CAD	154527	1154.146	2.5	43
RC-Inc-CAD	33	0.202	2.5.3	46
RC-Inc-ECCAD	33	0.202	2.5.3	46

Table 2.3: The Solotareff-3 problem with current technology — variable order $b \prec a \prec v \prec u$.

`full-cad` will construct a sign-invariant CAD of $\mathbb{R}^4$, as shown by the same cell counts as projection and lifting CAD with McCallum's projection operator: $54,037$ cells and $154,527$ cells. All of the options utilising a subset of QEPCAD's optimisations take just under five seconds (with around two seconds initialisation time), and constructing a full four-dimensional CAD takes six or eight seconds.

This proves the strength of the equational constraint and partial CAD techniques that QEPCAD can use, along with the practical time efficiency of its implementation.

Regular Chains CAD

Constructing a sign-invariant with the original regular chains algorithm (Section 2.5.2) produces the same number of cells as the McCallum projection and lifting algorithm and the unquantified `full-cad` CAD from QEPCAD: $54,037$ and $154,527$ cells (in both cases a single cell is found to be true, corresponding to the solution found by QEPCAD). The fact that these CADs are identical suggests that it may be the minimal sign-invariant CAD that can be algorithmically constructed.It takes around four to eight minutes to construct such a CAD, although it takes a substantial amount of additional time (one to twelve minutes) to construct representations of these cells to then count them (this is an implementational issue that the developers of `RegularChains` hope to eliminate).

Using the incremental regular chains algorithm (Section 2.5.3) will utilise all four equational constraints. This reduces the CAD down to 29 cells in 0.1-0.3 seconds, proving remarkably efficient.

Summary

The results in Tables 2.2 and 2.3 demonstrate the power of the various advances in CAD technology: projection operators, single equational constraints, partial CAD, regular chains algorithms, and utilising multiple equational constraints.

This example will be revisited in later chapters and compared to the results in Tables 2.2 and 2.3 to demonstrate how new advances in CAD theory can make existing technology more efficient. The results are summarised in Section 8.2.1 where Tables 8.1 and 8.2 demonstrate the power of the new theory given in this thesis.

2.13 Conclusion

In this chapter a thorough background of cylindrical algebraic decomposition was given. After the necessary background, the original algorithm from [Col75] was described along with many extensions. An alternative construction method by regular chains theory was also described in both a recursive and incremental form.

A discussion of the known complexity results for CAD showed that any algorithm will necessarily be doubly exponential in the number of variables. Alternatives to CAD were discussed with lower theoretical complexity (but not necessarily better practical performance) and some applications of CAD discussed. Finally, the Solotareff-3 example was discussed as a guiding example for the rest of the thesis.

Chapter 3

Truth Table Invariant CAD

Since their inception in 1975, the primary focus while constructing CADs has been the sign (or order) behaviour of the individual polynomials. This is generally more detail than needed, and nearly always results in a CAD that is more complex than necessary.

This chapter introduces a new invariance property for CAD, considering the truth values of quantifier-free formulae. A CAD satisfying this property is called truth-table invariant (a TTICAD) and is sufficient for applications of CAD.

When constructing a CAD by the original algorithm (and extensions) these ideas can be incorporated into the projection operator by a generalisation of equational constraints, although care has to be taken during the lifting phase. It is also possible to adapt the incremental regular chains CAD algorithm to incorporate TTICAD and it can be shown to be even more beneficial than TTICAD by projection and lifting.

Author's Contribution and Publication

The author contributed to various phases of the work in this chapter. Initial discussions between the author and Davenport instigated the idea of a TTICAD, which was then developed for a projection and lifting algorithm with the rest of the research group and McCallum. McCallum provided the proof of Theorem 3.3 and England provided the implementation of Algorithm 3.1, which the author then conducted the experimentation on. The remaining discussion and analysis was conducted by the entire research group.

The author was involved in the discussions of applying truth table invariance to regular chains with the rest of the research group, Chen, and Moreno Maza. The implementation was conducted by Chen and the proof of correctness by other members of the research group. The author conducted the experimentation and was involved in the discussion and investigation.

The discussion on extending to partial TTICAD is by the author. The work on branch cut analysis was mainly conducted by England (in collaboration with Cheb-Terrab of Maplesoft) and is presented as an application of TTICAD rather than original research.

The work in Sections 3.2 to 3.4 was published in [BDE+13] and submitted for publication in [BDE+14]. The work in Sections 3.5 to 3.7 was published in [BCD+14]. The work in Section 3.9 was published in [EBDW13] and [ECTB+14].

3.1 Motivation and Definition

When we consider a problem with cylindrical algebraic decomposition, we generally consider the sign-invariance of the polynomials. That is, on each cell in the CAD all polynomials are sign-invariant. This proves important for the construction of the CAD too, ensuring delineability in Collins' projection operator. Later McCallum [McC85] considered order-invariance to help the construction of CADs with his reduced projection operator. Order-invariance requires each polynomial to be sign-invariant on each cell and if the polynomial vanishes, then it does so to a constant order of vanishing.

Often what we are really concerned about is not the behaviour of polynomials, but rather the behaviour of formulae involving them. We first recall work by Brown [Bro98], which looked at truth invariance in CAD. We will discuss a motivating example that highlights the redundancies of standard CAD techniques and inspires the definition of a Truth Table Invariant CAD (TTICAD) that will be introduced in Section 3.1.3.

3.1.1 Truth-Invariant Cylindrical Algebraic Decompositions

Recall from Section 2.4.3 the definitions from [Bro98]:

Definition 3.1 ([Bro98])**.**
Let $\mathcal{A}$ and $\mathcal{B}$ be two CADs. We say $\mathcal{B}$ is **simpler** than $\mathcal{A}$ if $\mathcal{A}$ is a refinement of $\mathcal{B}$, i.e. each cell in $\mathcal{B}$ is the union of some cells of $\mathcal{A}$, and $\mathcal{A}$ and $\mathcal{B}$ are not equal.

Given a formula φ from the elementary theory of real closed fields, we say a CAD is **truth-invariant** with respect to the input formula if in each cell of the decomposition the formula is either identically true or identically false.

We will generalise the idea of truth-invariance to consider the invariance of a truth table for a collection of quantifier-free formulae.

3.1.2 Motivating Example

Let us consider an example to highlight some redundancies of sign-invariant projection and lifting CAD.

Example 3.1.
Consider finding the solutions to the following quantifier elimination problem:

$$\Omega : (\exists y) \left[x^2 + y^2 - 1 = 0 \wedge xy > \frac{1}{4} \right] \vee \left[\frac{x^2}{8} + y^2 = \frac{1}{2} \wedge x > y \right]. \tag{3.1}$$

We can pass this as input to QEPCAD and get the output:

$$x - 2 \leq 0 \wedge \left[2x + 1 > 0 \vee 16x^4 - 16x^2 + 1 < 0 \right]. \tag{3.2}$$

We can simplify (3.2) further to get the solution set as a simple half-open interval:

$$x \in \left(\frac{-\sqrt{6} - \sqrt{2}}{4},\ 2 \right].$$

Figures 3.1a and 3.1b show the full and partial CADs constructed by QEPCAD to solve this problem. It is clear that the CADs produced are more complicated than necessary to solve this problem: the two-dimensional CAD produced by the unquantified version of (3.1) constructs 465 cells.

Let us denote:

$$f_1 := x^2 + y^2 - 1; \quad g_1 := xy - \frac{1}{4}; \quad f_2 := \frac{x^2}{8} + y^2 - \frac{1}{2}; \quad g_2 := x - y;$$

so that Ω becomes simply $(\exists y)\,[f_1 = 0 \wedge g_1 > 0] \vee [f_2 = 0 \wedge g_2 > 0]$. Further let us denote:

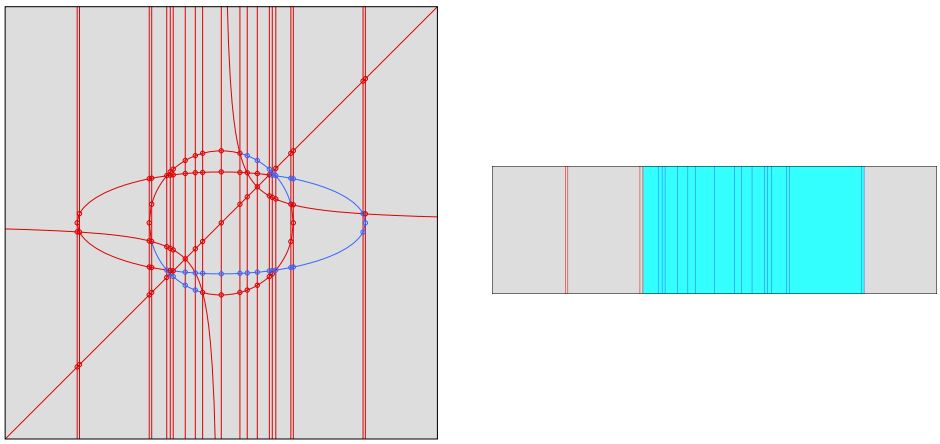
$$\omega_1 := [f_1 = 0 \wedge g_1 > 0]; \quad \omega_2 := [f_2 = 0 \wedge g_2 > 0]; \quad \omega := \omega_1 \vee \omega_2;$$

so that (3.1) becomes $(\exists y)\ \omega(x, y)$.

If attempting to solve Ω using CAD (utilising McCallum's projection operator) we would compute the following set of polynomials:

$$\left\{ \text{coeffs}_y(f), \text{disc}_y(f), \text{res}_y(f, \hat{f}) \mid f, \hat{f} \in \{f_1, g_1, f_2, g_2\}, f \neq \hat{f} \right\}; \tag{3.3}$$

for which there are 12 non-trivial polynomials describing 21 distinct solutions. This would therefore produce a CAD of $\mathbb{R}^1$ with 43 cells.



(a) 2D CAD produced by QEPCAD. (b) 1D CAD produced by QEPCAD.

Figure 3.1: CADs produced by QEPCAD for the motivating TTICAD example using the `p-2d-cad` command. Figure 3.1a was produced with the unquantified version of (3.1) to decompose the (x, y)-plane; Figure 3.1b was produced with the quantified version of (3.1) to decompose the (x)-plane (trivially expanded to two dimensions).

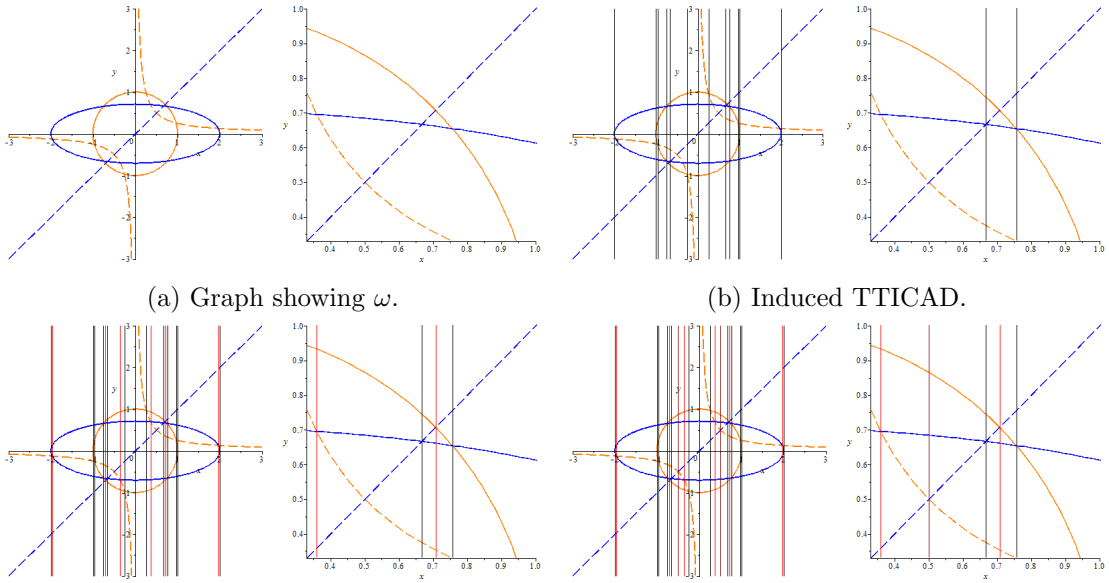
When determining the truth value of ω_1 (and similarly ω_2) we clearly only need to consider the behaviour of g_1 when $f_1 = 0$ is satisfied. This is exactly the observation that lead McCallum to formalise the idea of equational constraints in [McC99]. Therefore we need not include the full projection of g_1 in our set; we simply need to include $\text{res}_y(f_1, g_1)$ along with the projection of f_1 to determine the behaviour of ω_1.

Further, we do not need to worry about the interaction of g_1 with f_2 (similarly g_2 and f_1) as the only time when this interaction is important is when g_1 intersects f_2 *and* $f_1 = 0$ which is already covered by the inclusion of $\text{res}_y(f_1, g_1)$ and $\text{res}_y(f_1, f_2)$. Therefore we can use the following reduced projection set:

$$\Big\{\text{coeffs}_y(f_1), \text{coeffs}_y(f_2), \text{disc}_y(f_1), \text{disc}_y(f_2), \\ \text{res}_y(f_1, g_1), \text{res}_y(f_2, g_2), \text{res}_y(f_1, f_2)\Big\}. \quad (3.4)$$

There are only 12 distinct solutions to (3.4), producing a one-dimensional CAD with 25 cells. The omitted polynomials from (3.3) are:

$$\Big\{\text{coeffs}_y(g_1), \text{coeffs}_y(g_2), \text{disc}_y(g_1), \text{disc}_y(g_2), \\ \text{res}_y(f_1, g_2), \text{res}_y(f_2, g_1), \text{res}_y(g_1, g_2)\Big\}. \quad (3.5)$$



(a) Graph showing ω.

(b) Induced TTICAD.

(c) Induced implicit ECCAD ($f_1 f_2 = 0$).

(d) Induced sign-invariant CAD.

Figure 3.2: CADs produced by MAPLE for the motivating TTICAD example, Ω. A zoomed region ($(x, y) \in [\frac{1}{3}, 1]^2$) of each CAD is also given.

The solutions to (3.5) account for the remaining 9 solutions of (3.3).

Although ω does not contain an explicit equational constraint, it is clear that $f_1 \cdot f_2 = 0$ is an implied equational constraint and must be satisfied when ω is true. It can therefore be used with McCallum's equational constraint projection operator. This will produce the polynomials given in (3.4), however it will also include $\text{res}_y(f_1, g_2)$ and $\text{res}_y(f_2, g_1)$ as factors of $\text{res}_y(f_1 \cdot f_2, g_i)$.

Figure 3.2 shows the effect of using the various projection sets to construct a CAD. Figure 3.2a shows the polynomials involved in ω: the two ω_i are indicated in different colours, the f_i are indicated with solid lines, and the g_i are indicated with dashed lines. Figure 3.2b shows the effect of using the reduced projection set (3.4), which produces 177 cells in the final two-dimensional CAD. Figure 3.2c indicates projection with respect to the implied equational constraint $f_1 f_2 = 0$ and contains 269 cells. Finally, Figure 3.2d is created using the full McCallum projection set (3.3) which results in 465 cells (over 2.5 times the number of cells created by the reduced projection).

Note that Figure 3.2b is no longer a sign-invariant CAD for the polynomials in ω, nor is it invariant for the implied equational constraint $f_1 f_2 = 0$. However, the truth values of ω_1 and ω_2 are constant on every cell of the CAD, and so we call it a $\{\omega_1, \omega_2\}$-truth

table invariant CAD. We could now construct a truth table for ω_1 and ω_2 and divide the cells into each row from which we could describe any Boolean formula involving ω_1 and ω_2 (including, obviously, ω). This definition will be formalised in Section 3.1.3.

We now look more closely at a region of each of the CADs in Figure 3.2 to clarify the behaviour of the reduced projection set (3.4). The second graph in each subfigure of Figure 3.2 examines the CAD for the range $(x, y) \in [\frac{1}{3}, 1]^2$.

Figure 3.2a shows the polynomials for this region and it is clear there are multiple intersections, only some of which affect the behaviour of ω. Identifying only the x-values determined from the reduced projection set (3.4) in Figure 3.2b locates only two intersections: $x = \frac{2}{3}$ (where f_2 and g_2 intersect) and $x = \frac{2}{\sqrt{7}}$ (where f_1 and f_2 intersect). If we were to use the implied equational constraint $f_1 f_2 = 0$ we see in Figure 3.2c that we also identify $x = \frac{\sqrt{8-2\sqrt{14}}}{2}$ (where f_2 and g_1 intersect) and $x = \frac{1}{\sqrt{2}}$ (where f_1 and g_2 intersect). Finally, using the full projection set (3.3) in Figure 3.2d identifies $x = \frac{1}{2}$ (where g_1 and g_2) intersect.

The inclusion of each unnecessary solution creates a spurious point in the one-dimensional CAD, creating two additional cells and forces the inclusion of two stacks of cells in the CAD of $\mathbb{R}^2$. Therefore this simplification can have a huge effect on the number of cells produced in a final CAD. The TTICAD illustrated in Figure 3.2b can be used for any Boolean combination of ω_1 and ω_2, so it is still non-optimal for ω. Ideally, we would produce a CAD that is only truth-invariant for ω.

This example has demonstrated the power of reducing our projection set to obtain invariance for formulae rather than polynomials.

3.1.3 Definition

We now formalise this motivation into a definition of a new kind of invariance for CAD, related to truth-invariance, which will be the topic of this chapter.

Definition 3.2.
Let $\Phi := \{\varphi_i\}_{i=1}^t$ be a list of quantifier-free (Tarski) formulae. We say a cylindrical algebraic decomposition $\mathcal{D}$ is **truth table invariant** (a **TTICAD**), or more specifically **Φ-truth table invariant**, if the Boolean value of each φ_i is constant on each cell in $\mathcal{D}$.

Truth table invariance is a weaker condition than sign-invariance (which is itself weaker than order-invariance): if a CAD is sign-invariant with respect to all the polynomials in the φ_i then it will also be a TTICAD for Φ. However, if the φ_i are combined

into a, possibly quantified, formula φ then Φ-truth table invariance is a stronger condition than truth-invariance for φ. An algorithm will be given to produce TTICADs that are smaller than sign-invariant CADs for input lists of formulae. This will be achieved by generalising the theory of equational constraints suggested by Collins [Col98] and developed by McCallum [McC99].

In Sections 3.2 and 3.5, algorithms will be given to produce a TTICAD for a list of input formulae some of which contain an equational constraint. This will reduce the number of cells produced compared to a sign-invariant CAD.

As demonstrated in our motivating example, a TTICAD can be used for quantifier elimination. Given a quantified formula where the quantifier free part, φ, is decomposed into sub-formulae $\Phi := \{\varphi_i\}$, then a Φ-TTICAD can be constructed to facilitate quantifier elimination. Such a TTICAD would have fewer cells than a sign-invariant CAD and so the set of valid cells would likely be smaller. This will manifest itself in a simpler quantifier-free formula being output from the quantifier elimination algorithm (much like how a truth-invariant CAD produces a simpler formula [Bro98]).

A TTICAD can have other uses, and certain problems require truth-table invariance (where truth-invariance is insufficient). In Section 3.9 we will discuss the problem of decomposing complex space according to the branch cuts of a given formula. This can be used to validate algebraic simplification of elementary functions [BPB05, BBDP07, Phi11]. Representing each branch cut as a semi-algebraic set, a TTICAD can be produced to define the regions on which the simplification needs to be tested.

3.2 Projection and Lifting Algorithm

We present the reduced projection operator for TTICAD, followed by the algorithm to produce a TTICAD with this projection set.

3.2.1 Reduced Projection Operator

Previous work on Equational Constraints

Recall from Sections 2.4.1 and 2.32, McCallum's reduced projection set [McC85, McC98], and the theory of equational constraints [McC99], which we will generalise for the TTICAD operator.

The McCallum projection operator, ${}_{\mathbf{M}}\mathbf{P}$, is:

$$ {}_{\mathbf{M}}\mathbf{P}(A) := \{\text{coeffs}(f), \text{disc}_{x_n}(f), \text{res}_{x_n}(f,g) \mid f,g \in A, f \neq g\}\,. $$

We also assume that the standard trivial simplifications of removing constants and identical entries (up to a constant multiple). Most implementations also only include coefficients until the first constant coefficient.

The proof that ${}_{\mathbf{M}}\mathbf{P}$ is a valid projection operator relies on a key result. Recall that an order-invariant CAD requires polynomials to have constant order of vanishing on cells, as well as sign-invariance. Also we say that a set $A \subset \mathbb{Z}[\mathbf{x}]$ is an **irreducible basis** if the elements of A are of positive degree (in the main variable), irreducible, and pairwise relatively prime. The main result of [McC85, McC98] is Theorem 3.1:

Theorem 3.1 ([McC98, Theorem 1])**.**
Let A be an irreducible basis in $\mathbb{Z}[\mathbf{x}]$ and let S be a connected submanifold of $\mathbb{R}^{n-1}$. Suppose each element of ${}_{\mathbf{M}}\mathbf{P}(A)$ is order-invariant in S.

Then each element of A either vanishes identically on S or is analytic delineable on S [McC98, §3]. Further, the sections of A not identically vanishing are pairwise disjoint, and each element of A not identically vanishing is order-invariant in such sections.

Theorem 3.1 states that an order invariant CAD can be constructed from the projection polynomials in ${}_{\mathbf{M}}\mathbf{P}(A)$, as long as none of them vanish identically on a lower-dimensional cell. This motivates the following definition:

Definition 3.3.
A set A of n-variate integral polynomials, where $n \geq 1$, is said to be **well-oriented** if whenever $n > 1$ the following two conditions hold:

1). for every $f \in \text{prim}(A)$, $f(\alpha, x_n) = 0$ for at most a finite number of points $\alpha \in \mathbb{R}^{n-1}$;

2). ${}_{\mathbf{M}}\mathbf{P}(A)$ is well-oriented.

It is therefore possible to construct a CAD using McCallum's projection only if the input polynomials are well-oriented.

As mentioned in Sections 2.4.4 and 3.1, if an equational constraint is present in a formula then it can be used to simplify the projection set. If we have $f = 0$ as an equational constraint, then we need only worry about the behaviour of a non-equational constraint polynomial g when f vanishes. This behaviour is encoded in the resultant of f and g and Theorem 3.2 proves that replacing g with $\text{res}_{x_n}(f, g)$ is sufficient.

Theorem 3.2 ([McC99])**.**
Let $f(\mathbf{x})$, $g(\mathbf{x})$ be integral polynomials with positive degree in x_n, let $r(x_1, \ldots, x_{n-1})$ be their resultant, and suppose $r \neq 0$. Let S be a connected subset of $\mathbb{R}^{n-1}$ such that f is delineable on S and r is order-invariant on S.

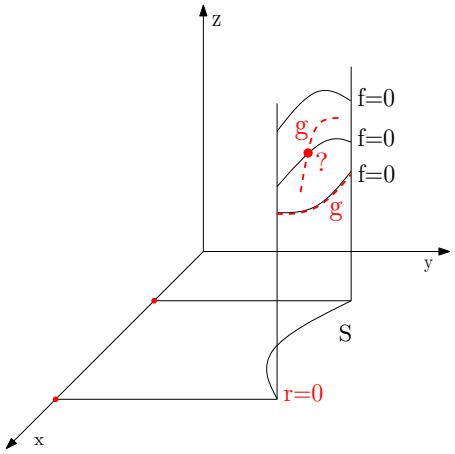


Figure 3.3: Graphical representation of Theorem 3.2. If f is delineable on S and r is order-invariant then g must either avoid or completely align with each section of f.

Then g is sign-invariant in every section f over S.

Figure 3.3 gives a graphical representation of Theorem 3.2 when working in three-dimensions. We assume that $f(x, y, z)$ and $g(x, y, z)$ have positive degree in z, and non-zero resultant, $r(x, y)$. We have S being any connected subset of $\mathbb{R}^2$ and assume that r is order-invariant on S. Assuming f is delineable over S we have three cases to consider, shown in Figure 3.3: f and g may not intersect; f and g may intersect but be distinct; or, f and g are identical over S.

Theorem 3.2 assures us that either f and g are disjoint over S (as in the top section of f in Figure 3.3), or they are completely aligned over S (as in the bottom section of f). Therefore, the situation in the middle section of f, where f and g intersect but are not identical over S, cannot happen.

Theorem 3.2 can be used to simplify the projection operator ${}_{\mathbf{M}}\mathbf{P}$. The equational constraint projection operator was first discussed in [Col98] and developed by McCallum in [McC99]. We consider a set of polynomials A, which contains a subset $E \subseteq A$: here, A represents all polynomials for a given problem, and E the equational constraints. We define the equational constraint projection set, ${}_{\mathbf{M}}\mathbf{P}_E(A)$, to be:

$$ {}_{\mathbf{M}}\mathbf{P}_E(A) := {}_{\mathbf{M}}\mathbf{P}(E) \cup \{\text{res}_{x_n}(f, g) \mid f \in E, g \in A, g \notin E\} . $$

This operator applies the full McCallum projection operator on the equational constraints polynomials, but does not do so for non-equational constraint polynomials. For any g that does not belong to E, it computes all cross-resultants with E but nothing

else. Theorem 3.2 allows us to use ${}_{\mathbf{M}}\mathbf{P}_E(A)$ for the first step of projection (followed by ${}_{\mathbf{M}}\mathbf{P}$) to construct a CAD invariant with respect to the equational constraint. As ${}_{\mathbf{M}}\mathbf{P}_E(A) \subseteq {}_{\mathbf{M}}\mathbf{P}(A)$ this should result in fewer cells being constructed.

Remark 3.1.
Theorem 3.2 is used to simplify the projection set, and thus the CAD of $\mathbb{R}^{n-1}$. It is worth noting that we can also use Theorem 3.2 to simplify the lifting operation from $\mathbb{R}^{n-1}$ to $\mathbb{R}^n$: we no longer need to lift with respect to g. This simplification in lifting is implemented within the `ProjectionCAD` package [Eng13b] and will be used in our TTICAD algorithm.

A TTICAD Projection Operator

We now consider how we can generalise the use of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ into the TTICAD projection operator.

We saw in Example 3.1 that given a list of formulae each of which has an individual equational constraint, we can apply ${}_{\mathbf{M}}\mathbf{P}_E(A)$ to each formula. We still need to be concerned with the interaction of the constraints, but can ignore behaviour of non-equational constraint polynomials away from the projections of their respective constraints. We formalise this idea.

As with [McC99], we first define our operator in the case of irreducible bases, which can then be generalised by considering contents and irreducible factors of the input sets of polynomials.

Let[1] $\mathcal{A} := \{A_i\}_{i=1}^t$ be a list of irreducible bases A_i and let $\mathcal{E} := \{E_i\}_{i=1}^t$ be a list of subsets $E_i \subseteq A_i$. Let $A := \bigcup_{i=1}^t A_i$ and $E := \bigcup_{i=1}^t E_i$.

Definition 3.4.
We define the **reduced projection of $\mathcal{A}$ with respect to $\mathcal{E}$**, denoted ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$, as:

$$ {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}) := \bigcup_{i=1}^{t} {}_{\mathbf{M}}\mathbf{P}_{E_i}(A_i) \cup \mathrm{RES}^{\times}(\mathcal{E}); $$

where $\mathrm{RES}^{\times}(\mathcal{E})$ is the cross-resultant set:

$$ \mathrm{RES}^{\times}(\mathcal{E}) := \left\{ \mathrm{res}_{x_n}(f, \hat{f}) \mid \exists\ i, j \text{ s.t. } f \in E_i, \hat{f} \in E_j, i < j, f \neq \hat{f} \right\}. $$

[1] To help keep track of various forms of input, we use the convention that uppercase Roman letters denote sets of polynomials and calligraphic letters denote lists of these sets.

Given a list of formulae $\Phi := \{\varphi_i\}_{i=1}^t$, we write $\mathbf{TTIP}(\Phi)$ to denote $\mathbf{TTIP}_{\mathcal{E}}(\mathcal{A})$ where each A_i is the irreducible basis for the polynomials in φ_i, and the sets E_i are those members of A_i corresponding to any equational constraints for φ_i.

To allow for easier comparison with the McCallum projection operator we formally define the set of polynomials we omit for each formula φ_i.

Definition 3.5.
We define the **excluded projection polynomials** of (A_i, E_i) to be:

$$\begin{aligned}\mathbf{Excl_{TTI}P}_{E_i}(A_i) &:= {}_{\mathbf{M}}\mathbf{P}(A_i) \setminus {}_{\mathbf{M}}\mathbf{P}_{E_i}(A_i) \\ &= \{\text{coeffs}_{x_n}(g), \text{disc}_{x_n}(g), \text{res}_{x_n}(g, \hat{g}) \mid g, \hat{g} \in A_i \setminus E_i, g \neq \hat{g}\}.\end{aligned}$$

Further, we can define the total set of excluded polynomials for $(\mathcal{A}, \mathcal{E})$:

$$\begin{aligned}\mathbf{Excl_{TTI}P}_{\mathcal{E}}(\mathcal{A}) &:= {}_{\mathbf{M}}\mathbf{P}(A) \setminus {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}) \\ &= \bigcup_{i=1}^{t} \mathbf{Excl_{TTI}P}_{E_i}(A_i) \quad \cup \\ &\qquad \{\text{res}_{x_n}(f, g) \mid \exists\, i, j \text{ s.t. } f \in E_i, g \in A_j, g \notin E, i \neq j\} \quad \cup \\ &\qquad\quad \{\text{res}_{x_n}(g, \hat{g}) \mid \exists\, i, j \text{ s.t. } g \in A_i, \hat{g} \in A_j, g, \hat{g} \notin E, i \neq j\}.\end{aligned}$$

We now provide the key theorem that proves that $\mathbf{TTIP}$ is a valid projection operator and will later be used to show that Algorithm 3.1 provides a truth-table invariant CAD.

Theorem 3.3 ([BDE+13])**.**
Let S be a connected submanifold of $\mathbb{R}^{n-1}$. Suppose each element of $\mathbf{TTIP}_{\mathcal{E}}(\mathcal{A})$ is order invariant in S.

Then the following hold:

- *each $f \in E$ either vanishes identically on S or is analytically delineable on S;*
- *the sections over S of the $f \in E$ which do not vanish identically are pairwise disjoint;*
- *each element $f \in E$ which does not vanish identically is order-invariant in such sections.*

Moreover, for each $1 \leq i \leq t$, every $g \in A_i \setminus E_i$ is sign-invariant in each section over S of every $f \in E_i$ which does not vanish identically.

Proof.
The crucial step for proving this result is observing that ${}_{\mathbf{M}}\mathbf{P}(E) \subseteq {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$. This is clear if we write:

$$ {}_{\mathbf{M}}\mathbf{P}(E) = \bigcup_{i=1}^{t} {}_{\mathbf{M}}\mathbf{P}(E_i) \cup \mathrm{RES}^{\times}(\mathcal{E}). $$

It is therefore a straightforward application of Theorem 3.1 to obtain the first three statements in this theorem.

The final statement requires the use of Theorem 3.2. Let i be in the range $1 \leq i \leq t$, $g \in A_i \setminus E_i$ and let $f \in E_i$. Suppose further that f does not vanish identically on S. As $\mathrm{res}_{x_n}(f, g)$ is contained in our projection set ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$, it must be order-invariant in S (by hypothesis). We have from the first statement in the theorem that f is delineable, and therefore by Theorem 3.2, g must be sign-invariant in each section of f over S.

□

This is a remarkably powerful theorem and it will be used to prove the correctness of our given algorithm. We will be able to apply it as long as no $f \in E$ vanishes identically on the lower-dimensional S. This will require a generalisation of Definition 3.3 relating to TTICAD.

Comparison of ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$ with other projection operators

It is clear that ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}) \subseteq {}_{\mathbf{M}}\mathbf{P}(A)$, with strict inclusion in all but the simplest case.

If all formulae $\{\varphi_i\}_{i=1}^{t}$ contain individual equational constraints, and are combined to form a larger parent formula φ, then the equational constraint projection operator can be used with an implied equational constraint consisting of $\prod_{f \in E} f = 0$. Using ${}_{\mathbf{M}}\mathbf{P}_E(A)$ with this equational constraint would avoid using the surplus coefficients, discriminants and cross-resultants involving just non-equational constraints. However, there would still be excess polynomials in the projection set: ${}_{\mathbf{M}}\mathbf{P}_E(A)$ contains all resultants

$$ \{\mathrm{res}_{x_n}(f_i, g_i) \mid f \in E_i, g \in A_j \setminus E_j, i \neq j, g \notin E\}. $$

These extra resultants describe the interaction of equational constraints with non-equational constraints from other formulae and therefore are unnecessary for truth table invariance with respect to $\{\varphi_i\}_{i=1}^{t}$.

Worked Example

We consider the projection sets for Example 3.1 to see clearly the differences in the various operators. We set $A_i := \{f_i, g_i\}$ and $E_i := \{f_i\}$ for $i = 1, 2$.

First, we use the TTICAD projection operator. We compute the reduced projection sets (with the necessary trivial simplifications) for each ω_i:

$$\begin{aligned} {}_{\mathbf{M}}\mathbf{P}_{E_1}(A_1) &= \left\{x^2 - 1, x^4 - x^2 + \frac{1}{16}\right\}; \\ {}_{\mathbf{M}}\mathbf{P}_{E_2}(A_2) &= \left\{x^2 - 4, 9x^2 - 4\right\}; \end{aligned}$$

and the single cross-resultant of the two equational constraints:

$$\mathrm{RES}^{\times}(\mathcal{E}) = \left\{\left(-\frac{7}{8}x^2 + \frac{1}{2}\right)^2\right\}.$$

The TTICAD projection set for this problem, ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$, is therefore the union of these three sets, which has 12 distinct solutions (Figure 3.2b).

As the two formulae are part of the larger $\omega = \omega_1 \vee \omega_2$, we can identify the implicit equational constraint, $f_1 f_2 = 0$. We can use McCallum's equational constraint projection operator, which would produce all the polynomials in ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$, along with the following two resultants:

$$\mathrm{res}_{x_n}(f_1, g_2) = 2x^2 - 1. \qquad \mathrm{res}_{x_n}(f_2, g_1) = \frac{1}{8}x^4 - \frac{1}{2}x^2 + \frac{1}{16}.$$

These polynomials produce an extra 6 distinct solutions to total 18 points (Figure 3.2c).

Finally, if we take the full McCallum projection set ${}_{\mathbf{M}}\mathbf{P}(A)$, we will have all the polynomials above but also gain the coefficients of g_1 and g_2 and their resultant. In this example, the only non-trivial coefficient is simply x, and the resultant is:

$$\mathrm{res}_{x_n}(g_1, g_2) = x^2 - \frac{1}{4}.$$

These additional polynomials provide 3 extra distinct solutions, totalling 21 points in the 1-dimensional CAD (Figure 3.2d).

This gives us a concrete demonstration of the difference in projection operators. As always, a simpler projection operator will produce a simpler CAD, but in the following section we will also discuss how simplified lifting can be used for ECCAD and TTICAD which will result in further savings.

3.2.2 A Projection and Lifting TTICAD Algorithm

We will now discuss, in detail, how the TTICAD projection operator can be used to construct a TTICAD. This algorithm was first given in [BDE+13] and later in [BDE+14].

Given an input of a list of quantifier-free formulae $\{\varphi_i\}_{i=1}^t$ in variables $x_1 \prec \cdots \prec x_n$ (where each φ_i has at least one equational constraint), Algorithm 3.1 produces a TTICAD of $\mathbb{R}^n$ (or **FAIL** if the input is not suited to the algorithm). We first discuss various details of the algorithm, before giving a proof of its correctness.

Algorithm 3.1 calls three subalgorithms which we briefly specify:

`sqfreebasis`: This computes a squarefree basis (Definition 2.4) of a set of polynomials to ensure they are primitive, squarefree, pairwise relatively co-prime. This procedure is implemented in most computer algebra systems.

`SplitR`: This is given in Algorithm 2.1, and decomposes one-dimensional real space according the roots of a set of polynomials. We assume that the output is given as a pair (I, S) of lists of cell indices and sample points.

`CADW`: This is an implementation of projection and lifting CAD as specified in [McC98] and given in Algorithm 2.4. We assume the output gives three outputs (as described in [McC98]), the first of which is a Boolean value w describing if the algorithm has been successful or not. If w is *true*, then the other two outputs are I and S: lists of cell indices and sample points.

We use the projection operator from Definition 3.4 in Algorithm 3.1, although care needs to be taken to ensure we obtain a valid output.

For an input list of formulae $\Phi = \{\varphi_i\}_{i=1}^t$ we first set A_i to be the set of all polynomials in φ_i, and put E_i to be the designated equational constraint polynomial $\{f_i\}$. We cannot simply apply the TTICAD projection operator (Definition 3.4) as we have no guarantee that the elements of each A_i are suitable.

We therefore extend Definition 3.4 by preprocessing our input (analogous to [McC99, §5]). We first remove the set of contents of all the elements of A, which we denote C. We take the finest squarefree bases of the primitive parts of the elements of the A_i and E_i, denoting them B_i and F_i, respectively. Then $\mathcal{B} = \{B_i\}_{i=1}^t$ and $\mathcal{F} = \{F_i\}_{i=1}^t$ satisfy the requirements for Definition 3.4, and so we create the set:

$$\mathfrak{P} := C \cup {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{F}}(\mathcal{B}).$$

Informally, for a general input $\Phi = \{\varphi_i\}_{i=1}^{t}$ when we write $\mathbf{TTI}\mathbf{P}(\Phi)$ or $\mathbf{TTI}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$ we mean this conditioned set $\mathfrak{P}$.

We will show that for appropriate input, Algorithm 3.1 will return a TTICAD for Φ. The condition that we use is a generalisation of well-orientedness (Definitions 2.26 and 3.3), which was given in [McC98] as a condition to ensure that `CADW` (implementing CAD using McCallum's improved projection operator, $\mathbf{M}\mathbf{P}$) provided valid input. The original definition requires the primitives of all polynomials to be nullified by at most a finite set of points, and for this condition to hold recursively for $\mathbf{M}\mathbf{P}$.

Definition 3.6.
We say that $\mathcal{A}$ is **(TTI)-well-oriented** with respect to $\mathcal{E}$ (and that Φ is **(TTI-)well-oriented**) if:

- for $n > 1$, every constraint polynomial f_i is nullified by at most a finite number of points in $\mathbb{R}^{n-1}$;
- $\mathbf{TTI}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$ (hence also $\mathfrak{P}$ in Algorithm 3.1) is well-oriented in the sense of Definitions 2.26 and 3.3 (as discussed in [McC85, McC98]).

We can now prove that Algorithm 3.1 behaves as specified.

Theorem 3.4 ([BDE+13])**.**
The output of Algorithm 3.1 is either a TTICAD of $\mathbb{R}^n$ for Φ (described by lists I and S of cell indices and sample points) or **FAIL** *(if Φ is not well oriented as specified in Definition 3.6).*

The proof is given in full in [BDE+13]. The proof consists of checking that **FAIL** will be returned for input that is not TTI-well-oriented, and otherwise that the output is truth table invariant. In the latter case we can apply Theorem 3.3 to $\mathcal{B}$, $\mathcal{F}$ and the cells of the $(n-1)$-dimensional CAD to get delineability of $\mathcal{F}$ and sign-invariance of $\mathcal{B}$ as required. The final step is to confirm that each formula is truth-invariant for the constructed CAD of $\mathbb{R}^n$.

With Theorem 3.4 we can now create TTICADs for lists of quantifier-free formulae, with each formula containing an equational constraint. We will discuss some extensions to Algorithm 3.1: the improved lifting it offers; avoiding **FAIL** when an equational constraint is nullified but the polynomials in $\text{Excl}_{\mathbf{TTI}\mathbf{P}_{E_i}}(A_i)$ are constant; and dealing with when there are quantifier-free formulae without an equational constraint. The latter in particular will allow TTICADs to be constructed for a much wider class of problems.

Algorithm 3.1: `TTICAD`$(\{\varphi_i\}_{i=1}^t, \texttt{vars})$: Standard truth table invariant CAD algorithm.

Input : A list of quantifier-free formulae $\{\varphi_i\}_{i=1}^t$; a list of ordered variables $vars = x_1 \prec \cdots \prec x_n$. Each formula φ_i should have a designated equational constraint $f_i = 0$.

Output: Either: a CAD $\mathcal{D}$ of $\mathbb{R}^n$ (described by lists I and S of cell indices and sample points) which is truth table invariant with respect to $\{\varphi_i\}_{i=1}^t$; or **FAIL** if the input is not well-oriented (Definition 3.6).

for $i = 1, \ldots, t$ **do**
  $E_i \leftarrow \{f_i\}$;
  $F_i \leftarrow \texttt{sqfreebasis}(\text{prim}(E_i))$; `// Preprocess equational constraints`
$F \leftarrow \bigcup_{i=1}^t F_i$;
if $n = 1$ **then**
  $(I, S) \leftarrow \texttt{SplitR}(\texttt{F})$;
  return (I, S) to represent $\mathcal{D}$; `// Base case`
else
  for $i = 1, \ldots, t$ **do**
    $A_i \leftarrow \text{polys}(\varphi_i)$;
    $C_i \leftarrow \text{cont}(A_i)$;
    $B_i \leftarrow \texttt{sqfreebasis}(\text{prim}(A_i))$; `// Preprocess polynomials`
  $C \leftarrow \bigcup_{i=1}^t C_i$; $\mathcal{B} \leftarrow \{B_i\}_{i=1}^t$; $\mathcal{F} \leftarrow \{F_i\}_{i=1}^t$;
  $\mathfrak{P} \leftarrow C \cup {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{F}}(\mathcal{B})$; `// Projection set`
  $(w', I', S') \leftarrow \texttt{CADW}(n-1, \mathfrak{P})$; `// (n − 1)-dimensional CAD`
  if $w' = \text{false}$ **then**
    return FAIL; `// 𝔓 is not well oriented`
  $I \leftarrow \varnothing$; $S \leftarrow \varnothing$;
  for $c' \in \mathcal{D}'$ **do**
    $L_c \leftarrow \varnothing$;
    for $i = 1, \ldots, t$ **do**
      if $\exists f \in E_i$ *which is nullified on* c **then**
        if $\dim(c) > 0$ **then**
          return FAIL; `// {φ_i}_{i=1}^t is not well oriented`
        else
          $L_c \leftarrow L_c \cup B_i$;
      else
        $L_c \leftarrow L_c \cup F_i$;
    $(I_c, S_c) \leftarrow \texttt{GenerateStack}(L_c, x_n, c)$; `// Lifting phase`
    $I \leftarrow I \cup I_c$; $S \leftarrow S \cup S_c$;
  return (I, S) to represent $\mathcal{D}$;

Improved Lifting

We mentioned when discussing Theorem 3.2, that it allows for simpler lifting as well as a simpler projection set. Theorem 3.2 states that the non-equational constraints are sign-invariant on the sections of the equational constraint, which are the only cells on which the formula can be satisfied. Therefore there is no need to lift with respect to the non-constraint polynomials, and so we generally[2] lift only with respect to the equational constraints.

Note that we are able to do this as we only need sign-invariance to deduce the truth value of the φ_i. If we were at a lower level in the CAD (and so needed order-invariance to apply Theorems 3.1 or 3.2) or required global order-invariance then this step would be invalid.

If we use Algorithm 3.1 with a single formula $\Phi = \{\varphi_1\}$ then we emulate McCallum's equational constraint theory [McC99]. However, this improved lifting has been unexploited until now, meaning that we will often get a simpler CAD than using current implementations of equational constraint CAD such as QEPCAD.

Avoiding FAIL when $\mathbf{Excl_{TTI}P}$ is constant

In [Bro05b] it was pointed out that there are cases when input to a CAD algorithm utilising McCallum's projection operator (without equational constraints) is not well-oriented but an order-invariant CAD can still be produced.

When constructing a TTICAD using Algorithm 3.1 there are also cases when non-well oriented input can still be used to create a TTICAD. The following result allows Algorithm 3.1 to sometimes avoid failure when an equational constraint vanishes identically on a positive-dimensional cell.

Lemma 3.5 ([BDE+14])**.**
Let f_i be an equational constraint which vanishes identically on a cell $c' \in \mathcal{D}'$ constructed in Algorithm 3.1 (line 15). If all the polynomials in $\mathbf{Excl_{TTI}P}_{E_i}(A_i)$ are constant on c', then any $g \in A_i \setminus E_i$ will be delineable over c'.

This result allows for an implementation of Algorithm 3.1 to avoid returning **FAIL** in more cases. This could be extended to include cases where the elements of $\mathbf{Excl_{TTI}P}_{E_i}(A_i)$ do not have any real roots in the cell c' (and so are viewed as constant on that cell) but this check could be rather substantial and it may be quicker to use a different CAD theory.

[2]The only exception is if f_i is nullified on a zero-dimensional cell at which point we simply lift with respect to all non-equational constraints.

3.2.3 Dealing with Clauses Without an Equational Constraint

It is obviously limiting that Algorithm 3.1 requires all the quantifier-free formulae to have an (explicit) equational constraint, and this prevents its application to many problems. It is possible to adapt Algorithm 3.1 to deal with the case that some of the quantifier-free formulae do not have an equational constraint: in short, all polynomials in that formula are given the prominence that an equational constraint polynomial is given in Algorithm 3.1.

This extension is shown in Algorithm 3.2. It is clear that Algorithm 3.2 terminates, and all that remains is to show that it is correct.

Theorem 3.6 ([BDE+14])**.**
The output of Algorithm 3.2 is either a TTICAD of $\mathbb{R}^n$ for Φ (described by lists I and S of cell indices and sample points) or **FAIL** *(if Φ is not well oriented as specified in Definition 3.6).*

The proof is given in full in [BDE+14] and consists of checking the addition of the if-statement resulting in the assignment of E_i on lines 3 and 5 ensures truth-invariance for formulae without equational constraints.

3.2.4 Worked Example

Let us consider Example 3.1 to demonstrate the power of Algorithms 3.1 and 3.2.

We begin by constructing a TTICAD for Ω using Algorithm 3.1. Our input is the set of formulae:

$$\Omega = \{\omega_1, \omega_2\} = \{[f_1 = 0 \wedge g_1 > 0], [f_2 = 0 \wedge g_2 > 0]\}.$$

Computing a TTICAD for this example (using Algorithm 3.1 or 3.2) was shown to construct 177 cells, whilst a CAD with respect to the implicit equational constraint $(f_1 f_2 = 0)$ produces 269 cells, and the full sign-invariant CAD contains 465 cells.

We now consider constructing the TTICAD for $\Omega^\dagger$ (for which Algorithm 3.1 is not applicable):

$$\Omega^\dagger = \{\omega_1^\dagger, \omega_2^\dagger\} = \{[f_1 = 0 \wedge g_1 > 0], [f_2 > 0 \wedge g_2 > 0]\}.$$

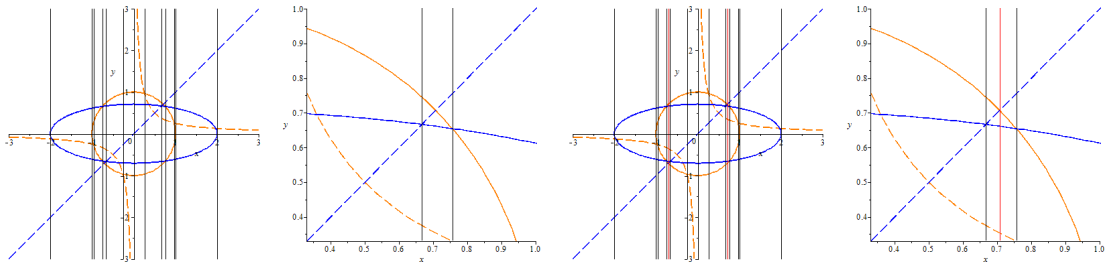
Applying Algorithm 3.2 to $\Omega^\dagger$ produces extra polynomials: $\text{disc}_y(g_2)$ and $\text{res}_y(f_1, g_2)$. The first is trivial, whilst the latter is $2x^2 - 1$ so identifies two extra points in the one-dimensional CAD. Further, the set of polynomials that is used for lifting consists of $\{f_1, f_2, g_2\}$ rather than just $\{f_1, f_2\}$. This results in 263 cells. In this case there is no

Algorithm 3.2: `TTICAD`$(\{\varphi_i\}_{i=1}^t, \texttt{vars})$: Extended truth table invariant CAD algorithm.

Input : A list of quantifier-free formulae $\{\varphi_i\}_{i=1}^t$; a list of ordered variables $vars = x_1 \prec \cdots \prec x_n$. Each formula φ_i may or may not have a designated equational constraint $f_i = 0$.

Output: A generic CAD, D, for F

for $i = 1, \ldots, t$ **do**
  if φ_i *has a designated equational constraint* $f_i = 0$ **then**
    $E_i \leftarrow \{f_i\}$;
  else
    $E_i \leftarrow A_i$;
  $F_i \leftarrow$ `sqfreebasis`$(\text{prim}(E_i))$; `// Preprocess equational constraints`
$F \leftarrow \bigcup_{i=1}^t F_i$;
if $n = 1$ **then**
  $(I, S) \leftarrow$ `SplitR`$(\texttt{F})$;
  return (I, S) to represent $\mathcal{D}$; `// Base case`
else
  for $i = 1, \ldots, t$ **do**
    $A_i \leftarrow \text{polys}(\varphi_i)$;
    $C_i \leftarrow \text{cont}(A_i)$;
    $B_i \leftarrow$ `sqfreebasis`$(\text{prim}(A_i))$; `// Preprocess polynomials`
  $C \leftarrow \bigcup_{i=1}^t C_i$; $\mathcal{B} \leftarrow \{B_i\}_{i=1}^t$; $\mathcal{F} \leftarrow \{F_i\}_{i=1}^t$;
  $\mathfrak{P} \leftarrow C \cup {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{F}}(\mathcal{B})$; `// Projection set`
  $(w', I', S') \leftarrow$ `CADW`$(n-1, \mathfrak{P})$; `// (n-1)-dimensional CAD`
  if $w' = \text{false}$ **then**
    return FAIL
  ; `// 𝔓 is not well oriented`
  $I \leftarrow \varnothing$; $S \leftarrow \varnothing$;
  for $c' \in \mathcal{D}'$ **do**
    $L_c \leftarrow \varnothing$;
    for $i = 1, \ldots, t$ **do**
      if $\exists f \in E_i$ *which is nullified on* c **then**
        if $\dim(c) > 0$ **then**
          return FAIL; `// {φ_i}_{i=1}^t is not well oriented`
        else
          $L_c \leftarrow L_c \cup B_i$;
      else
        $L_c \leftarrow L_c \cup F_i$;
    $(I_c, S_c) \leftarrow$ `GenerateStack`(L_c, x_n, c); `// Lifting phase`
    $I \leftarrow I \cup I_c$; $S \leftarrow S \cup S_c$;
  return (I, S) to represent $\mathcal{D}$;



(a) Induced TTICAD for Ω (b) Induced TTICAD for $\Omega^\dagger$

Figure 3.4: TTICADs produced by MAPLE for Ω and $\Omega^\dagger$ in the motivating TTICAD example. A zoomed region ($(x, y) \in [\frac{1}{3}, 1]^2$) of the TTICADs produced is also shown.

implicit equational constraint and so the only other sufficient CAD is the sign-invariant CAD (with 465 cells).

3.3 Implementation and Experimentation: Projection and Lifting TTICAD

We discuss the implementation of Algorithms 3.1 and 3.2 and experimental results displaying their efficacy.

3.3.1 Implementation of TTICAD by Projection and Lifting

To correctly implement an instance of Algorithms 3.1 and 3.2 a CAD needs to be produced that is order-invariant with respect to its input (to ensure the CAD produced on line 15 is suitable). We use the implementation of `CADW` in `ProjectionCAD` (the `CADFull` procedure with `method=McCallum`). Advances in the `RegularChains package` since this work was submitted for publication, such as shifting computation of resultants into kernel commands, has shown a substantial speed up in all the `ProjectionCAD` code. For this reason, the tests from [BDE+13] and [BDE+14] have been updated with new results (although the conclusions are identical).

The implementation of TTICAD is non-optimised and its purpose is not to illustrate the speed of TTICAD (although this proves competitive in many cases), but to demonstrate the power of the theory. The number of cells in the TTICAD produced is of more interest, and is directly correlated to the construction time. The hope is that in the future a more optimised implementation of TTICAD can be created (perhaps within another optimised system, like QEPCAD) and TTICADs can be constructed even faster.

3.3.2 Experimental Results for TTICAD by Projection and Lifting

To demonstrate the power of the TTICAD theory we compute TTICADs for a collection of examples, providing both cell counts and timings. To provide a context for these results we also compute CADs using a variety of techniques. The PL-CAD column is computed using the projection and lifting algorithm described in [McC85, McC98] using McCallum's projection operator. The QEPCAD column refers to constructing a CAD using QEPCAD-B using the options `+N500000000` and `+L200000` and with initialisation included in the timings. To allow QEPCAD to perform to its full strength, we declare any explicit equational constraints (so it can use the theory outlined in [McC99]) if present, or declare the implicit equational constraint (the product of the equational constraints for the individual quantifier-free formulae) if all formulae contain an equational constraint. The MATHEMATICA column refers to using the `CylindricalDecomposition` command which does not produce a CAD, but rather a cylindrical algebraic formula (CAF) which is constructed from one [Str12]. The author of MATHEMATICA's command kindly provided cell counts for the problems, although it should be noted that the use of meta-algorithms in MATHEMATICA means that there is not a guarantee that a CAD was ever constructed (for example, with a conjunction of equations MATHEMATICA will automatically just compute a Gröbner basis).

The examples we consider are from a range of sources and we use a suffix of A/B to illustrate different variable orderings for a single problem. We use examples from [BH91], adapted to be suited for TTICAD by changing certain conjunctions into disjunctions, and denote such new problems with †. We then provide two examples (Kahan and Arcsin) sourced from the application of branch cut analysis for simplification (see Section 3.9 for further details). We consider some worked examples from [BDE$^+$13] and [BDE$^+$14] and also a small collection of randomly generated examples: disjunctions of two quantifier free formulae, only one of which has an equational constraint, using random polynomials in three variables of degree at most two. All examples are given in the CAD repository described in [WBD13] and Appendix B.

The experimental results are given in Table 3.1. For each problem, along with the name (as used in [WBD13]) and experimental results, we give the number of variables n, the maximum degree of polynomials involved d, and the number of quantifier free formula used for TTICAD t.

First we compare TTICAD with a sign-invariant CAD produced using the `ProjectionCAD` module with McCallum's projection operator. As the `TTICAD` and `CADFull` commands are both implemented in the same architecture this gives us a direct comparison

Problem		PL-CAD		TTICAD		QEPCAD		MAPLE		MATHEMATICA	
Name	n d t	Time	Cells	Time	Cells	Time	Cells	Time	Cells	Time	Cells
IntersectionA	3 2 1	360.1	3707	1.7	269	4.5	825	—	Err	0.0	3
IntersectionB	3 2 1	332.2	2985	1.5	303	4.5	803	50.2	2795	0.0	3
RandomA	3 3 1	268.5	2093	4.5	435	4.6	1667	23.0	1267	0.1	657
RandomB	3 3 1	442.7	4097	8.1	711	5.4	2857	48.1	1517	0.0	191
Intersection†A	3 2 2	360.1	3707	68.7	575	4.8	3723	—	Err	0.1	601
Intersection†B	3 2 2	332.2	2985	70.0	601	4.7	3001	50.2	2795	0.1	549
Random†A	3 3 2	268.5	2093	223.4	663	4.6	2101	23.0	1267	0.2	808
Random†B	3 3 2	442.7	4097	268.4	1075	142.4	4105	48.1	1517	0.2	1156
Ellipse†A	5 4 2	—	**F**	—	**F**	291.6	500609	1940.1	81193	11.2	80111
Ellipse†B	5 4 2	T/O	—	T/O	—	T/O	—	T/O	—	2911.2	16603131
Solotareff†A	4 3 2	677.6	54037	46.1	**F**	4.9	20307	1014.2	54037	0.1	260
Solotareff†B	4 3 2	2009.2	154527	123.8	**F**	6.3	87469	2951.6	154527	0.1	762
Collision†A	4 4 2	264.6	8387	267.7	8387	5.0	7813	376.4	7895	3.6	7171
Collision†B	4 4 2	—	Err	—	Err	T/O	—	T/O	—	591.5	1234601
KahanA	2 4 7	10.7	409	0.3	55	4.8	261	15.2	409	0.0	72
KahanB	2 4 7	87.9	1143	0.3	39	4.8	1143	154.9	1143	0.1	278
ArcsinA	2 4 4	2.5	225	0.3	57	4.6	225	3.3	225	0.0	175
ArcsinB	2 4 4	6.5	393	0.2	25	4.5	393	7.8	393	0.0	79
2DEx(Φ)A	2 2 2	5.7	317	1.2	105	4.7	249	6.3	317	0.0	24
2DEx(Φ)B	2 2 2	6.1	377	1.5	153	4.5	329	7.2	377	0.0	175
2DEx(Ψ)A	2 2 2	5.7	317	1.6	183	4.9	317	6.3	317	0.1	372
2DEx(Ψ)B	2 2 2	6.1	377	1.9	233	4.8	377	7.2	377	0.1	596
3DExA	3 3 2	3795.8	5453	5.0	109	5.3	739	—	Err	0.1	44
3DExB	3 3 2	3404.7	6413	5.8	153	5.7	1009	—	Err	0.1	135
Random1	3 2 2	16.4	1533	76.8	1533	4.9	1535	25.7	1535	0.2	579
Random2	3 2 2	837.9	7991	132.4	2911	5.2	8023	173.0	8023	0.8	2551
Random3	3 2 2	258.6	8889	98.1	4005	5.3	8913	77.9	5061	0.7	3815
Random4	3 2 2	1442.3	11979	167.1	4035	5.4	12031	258.3	12031	1.3	4339
Random5	3 2 2	310.3	11869	110.7	4905	5.5	11893	104.3	6241	0.9	5041

Table 3.1: Comparing TTICAD (by Projection and Lifting) to the full CAD built with the same architecture and other CAD algorithms (taken from [BDE+13, BDE+14]).

and clearly shows the benefit of the TTICAD theory.

We can see clearly that in all cases where both `TTICAD` and `CADFull` run successfully the cell count for TTICAD is less than or equal to that of a sign-invariant CAD. This confirms the fact that each cell of a TTICAD is a superset of cells from the sign-invariant CAD produced by `CADFull`. In fact, the only examples where the cell counts are equal are Collision†A and Random 1, in which the non-equational constraints are simple enough that the projection polynomials remain unchanged.

This comparison also illustrates the drawback of the TTICAD theory - for Solotareff † A/B the problem is not TTI-well-oriented so the TTICAD algorithm returns **FAIL**, but the problem is well-oriented in the McCallum CAD sense (Definitions 2.26 and 3.3) and so `CADFull` returns a valid CAD.

We can see that a truly impressive reduction in cell count can occur: in the 3D worked example from [BDE+14] a 50-fold reduction in cell count (and a 759-fold reduction in time) occurs.

We can perform some basic statistical analysis on these results to illustrate the power of TTICAD. Of all the cases where both `TTICAD` and `CADFull` run successfully we can compute the reduction in cell counts. On average for our data set, a TTICAD offers a 68.6% reduction the size of a sign-invariant CAD, and on average reduces the time to

construct the CAD by 59.1%.

Comparing TTICAD with QEPCAD, the `CylindricalAlgebraicDecompose` algorithm in MAPLE 16 (RC-Rec-CAD described in Section 2.5.2), or MATHEMATICA is a little less straightforward, as they are based on different implementations and algorithms. QEPCAD utilises partial CAD techniques, and MATHEMATICA produces cylindrical algebraic formulae (as opposed to a decomposition) but TTICAD proves to be competitive. For the 24 examples where both TTICAD and QEPCAD complete, all but Collision†A give a lower cell count with TTICAD. However QEPCAD can construct three CADs (Ellipse†A and Solotareff†A/B) that are not well-oriented with respect to TTICAD, and can be quicker than TTICAD for some examples (even with a larger cell count) thanks to its optimised implementation. TTICAD performs similarly against MAPLE 16's `CylindricalAlgebraicDecompose`, producing smaller cell counts in all except Collision†A but with MAPLE successfully constructing a CAD for the non-well-oriented examples and occasionally being quicker than TTICAD. MATHEMATICA is quicker for all examples (and is the only algorithm to successfully complete for all problems), which is to be expected, but TTICAD can offer lower cell counts for just over half the examples.

Number of Quantifier-Free Formulae

It would seem clear that as the number of quantifier-free formulae in a problem increases, the benefit of TTICAD theory should become more pronounced (assuming at least one formula has an equational constraint). As the number of formulae increases, there will be many more inter-formula resultants when computing a sign-invariant CAD, of which a large proportion will be ignored due to TTICAD theory. To illustrate this saving experimentally we consider the following set of examples, which has been extended from [BDE+14].

Example 3.2.
Assume that $x \prec y$, and define the following set of examples for any $j \in \mathbb{N}$:

$$f_j := (x-4j)^2 + (y-j)^2 - 1; \quad g_j := (x-4j)\cdot(y-j) - \frac{1}{4};$$
$$F_j := \{f_k, g_k \mid 0 \leq k \leq j\};$$
$$\Phi_j := \bigvee_{k=0}^{j} (f_k = 0 \wedge g_k < 0); \quad \Psi_j := \left(\bigvee_{k=0}^{j-1} (f_k = 0 \wedge g_k < 0)\right) \vee (f_j < 0 \wedge g_j < 0).$$

Note that Φ_1 and Ψ_1 are the worked examples from [BDE+13, BDE+14]. Successive

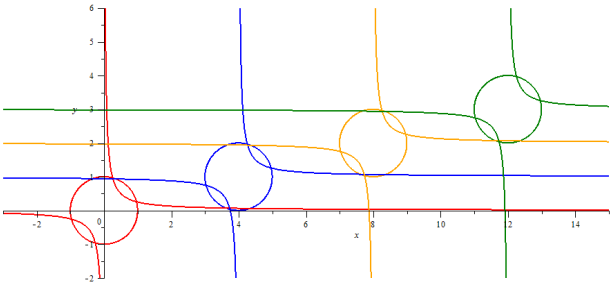


Figure 3.5: The polynomials in F_3 for Φ_3 and Ψ_3 in Example 3.2

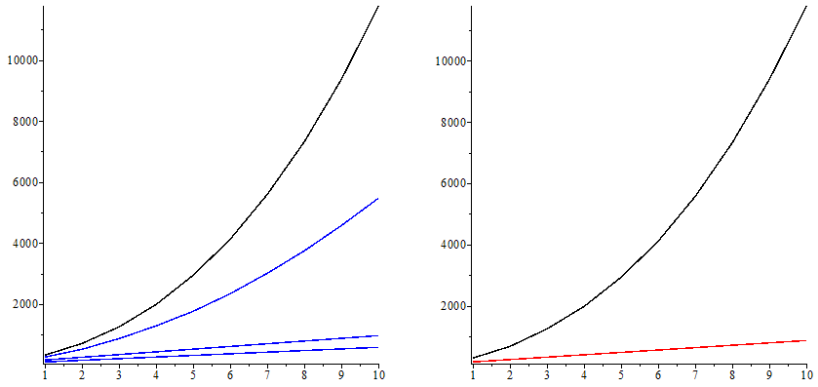
j	F_j	Φ_j			Ψ_j	
	`CADFull`	`ECCAD`	`TTICAD`	QEPCAD	`TTICAD`	QEPCAD
1	317	145	105	249	183	317
2	695	237	157	509	259	695
3	1241	329	209	849	335	1241
4	1979	421	261	1269	411	1979
5	2933	513	313	1769	487	2933
6	4127	605	365	2349	563	4127
7	5585	697	417	3009	639	5585
8	7331	789	469	3749	715	7331
9	9389	881	521	4569	791	9389
10	11783	973	573	5469	867	11783

Table 3.2: Cell counts for various CADs constructed for Example 3.2.

Φ_j and Ψ_j are generalisations: Φ_j is a disjunction of $j+1$ formulae each containing an equational constraint; Ψ_j is a disjunction of j formulae each containing an equational constraint, and one formula without an equational constraint (therefore requiring Algorithm 3.2). The polynomials in F_3 for Φ_3 and Ψ_3 are shown in Figure 3.5.

Table 3.2 shows the cell counts of CADs for F_j, Φ_j and Ψ_j with a variety of methods. The `CADFull` column constructs a sign-invariant CAD with `ProjectionCAD` with McCallum's projection operator; the `ECCAD` column constructs a CAD with `ProjectionCAD` according to the implicit equational constraint of Φ_j; the `TTICAD` column constructs a TTICAD with `ProjectionCAD` for Φ_j and Ψ_j according to Algorithms 3.1 and 3.2, respectively; the QEPCAD column constructs a CAD with QEPCAD-B, declaring the implicit equational constraint for Φ_j.

Figure 3.6 shows the difference in CAD growth for the various problems. In Figure 3.6a the cell counts for Φ_j are plotted for, from top to bottom: `CADFull`, QEPCAD, `ECCAD`, and `TTICAD`. In Figure 3.6b the cell counts for Ψ_j are plotted for, from top to bottom: `CADFull`/QEPCAD, and `TTICAD`. It is clear that the size of the sign-invariant



(a) Cell counts for Φ_j (b) Cell counts for Ψ_j

Figure 3.6: Cell counts for Φ_j and Ψ_j with `TTICAD`, `ECCAD` (implicit equational constraint), QEPCAD (implicit equational constraint), and `CADFull` (McCallum's projection operator.

CAD constructed with `CADFull` or QEPCAD is growing at a much faster rate than `TTICAD` or `ECCAD` with an increase in the number of formulae.

We can explicitly describe this growth behaviour, which we list in increasing order of growth:

- `TTICAD` Φ_j: Linear growth described by $52j + 53$;
- `TTICAD` Ψ_j: Linear growth described by $76j + 107$;
- `ECCAD` Φ_j: Linear growth described by $92j + 53$;
- QEPCAD Φ_j: Quadratic growth described by $40j^2 + 140j + 69$;
- `CADFull` F_j: Cubic growth described by $4j^3 + 60j^2 + 170j + 83$ (this is the same behaviour as QEPCAD on Ψ_j).

These results are perhaps unsurprising if we consider the problem at hand. The inclusion of another formula to Φ_j when using TTICAD simply decomposes the rightmost cylinder according to the circle and the points intersecting the hyperbola. Adding another formula to Ψ_j requires the entire hyperbola to be considered, but it only intersects one other equational constraint (the circle to its immediate left) so again there is only a linear effect.

Considering the set of polynomials F_j, we are increasing the number of polynomials, but keeping the degree, norm length, and number of variables fixed. The complexity results discussed in Section 2.6 show that with a fixed number of variables the complexity

bounds are polynomial in the number of polynomials, degree, and norm length, which correlates with this behaviour. We can also see in Figure 3.5 that adding an extra formula will intersect all previous hyperbolas, as well as the last and penultimate circles, which explains the non-linear polynomial behaviour.

3.4 Further Ideas and Extensions: Projection and Lifting TTICAD

3.4.1 ResCAD

We introduce an intuitive way to think of TTICAD construction, which aligns with the output of Algorithm 3.1 under specific conditions.

Definition 3.7.
Let $\Phi = \{\varphi_i\}_{i=1}^t$ be a collection of quantifier free formulae. Let A_i be the set of polynomials in φ_i and let E_i be a non-empty subset of A_i. Define the **ResCAD set** of Φ, denoted $\mathcal{R}(\Phi)$, to be:

$$\mathcal{R}(\Phi) := E \cup \bigcup_{i=1}^{t} \{\text{res}_{x_n}(f, g) \mid f \in E_i, g \in A_i \setminus E_i\}.$$

We can see the relation between the ResCAD set and the TTICAD projection operator in the following theorem.

Theorem 3.7.
Let $\Phi = \{\varphi_i\}_{i=1}^t$ be a collection of quantifier free formulae. Let $\mathcal{A} = \{A_i\}_{i=1}^t$ be a collection of irreducible bases for the polynomials in each φ_i, and let $\mathcal{E} = \{E_i\}_{i=1}^t$ be a collection of non-empty subsets $E_i \subseteq A_i$.

Then the following relation holds:

$$_{\mathbf{M}}\mathbf{P}\left(\mathcal{R}(\Phi)\right) = {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}).$$

Proof.
For each pair of sets (A_i, E_i) we define:

$$\mathcal{R}_{x_n}(E_i, A_i) = \{\text{res}_{x_n}(f, g) \mid f \in E_i, g \in A_i \setminus E_i\},$$

so that we can write the ResCAD set as

$$\mathcal{R}(\Phi) = E \cup \bigcup_{i=1}^{t} \mathcal{R}_{x_n}(E_i, A_i).$$

Consider ${}_{\mathbf{M}}\mathbf{P}(\mathcal{R}(\Phi))$. We first note that for every i, the set $\mathcal{R}_{x_n}(E_i, A_i)$ consists only of resultants taken with respect to x_n. As such, no polynomial in $\mathcal{R}_{x_n}(E_i, A_i)$ can have positive degree in x_n. So, according to the `CADW` algorithm, they are simply passed down to the next level of projection. Therefore we can write

$${}_{\mathbf{M}}\mathbf{P}(\mathcal{R}(\Phi)) = {}_{\mathbf{M}}\mathbf{P}(E) \cup \bigcup_{i=1}^{t} \mathcal{R}_{x_n}(E_i, A_i).$$

We now rewrite ${}_{\mathbf{M}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$ using the definition of ${}_{\mathbf{M}}\mathbf{P}_{E}(A)$:

$$\begin{aligned}
{}_{\mathbf{M}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}) &= \bigcup_{i=1}^{t} {}_{\mathbf{M}}\mathbf{P}_{E_i}(A_i) \cup \mathrm{RES}^{\times}(\mathcal{E}) \\
&= \bigcup_{i=1}^{t} [{}_{\mathbf{M}}\mathbf{P}(E_i) \cup \mathcal{R}_{x_n}(E_i, A_i)] \cup \mathrm{RES}^{\times}(\mathcal{E}) \\
&= \left[\bigcup_{i=1}^{t} {}_{\mathbf{M}}\mathbf{P}(E_i) \cup \mathrm{RES}^{\times}(\mathcal{E})\right] \cup \bigcup_{i=1}^{t} \mathcal{R}_{x_n}(E_i, A_i).
\end{aligned}$$

Therefore it is sufficient to prove that

$${}_{\mathbf{M}}\mathbf{P}(E) = \bigcup_{i=1}^{t} {}_{\mathbf{M}}\mathbf{P}(E_i) \cup \mathrm{RES}^{\times}(\mathcal{E}).$$

Recall for a set F of polynomials

$${}_{\mathbf{M}}\mathbf{P}(F) = \{\mathrm{coeffs}(f), \mathrm{disc}_{x_n}(f) \mid f \in F\} \cup \{\mathrm{res}_{x_n}(f, f') \mid f, f' \in F, f \neq f'\}.$$

Now we can rewrite ${}_{\mathbf{M}}\mathbf{P}(E)$ as follows:

$$\begin{aligned}
{}_{\mathbf{M}}\mathbf{P}(E) &= {}_{\mathbf{M}}\mathbf{P}\left(\bigcup_{i=1}^{t} E_i\right) \\
&= \bigcup_{i=1}^{t} \{\mathrm{coeffs}(f), \mathrm{disc}_{x_n}(f) \mid f \in E_i\} \cup \{\mathrm{res}_{x_n}(f, f') \mid f, f' \in E, f \neq f'\}. \quad (3.6)
\end{aligned}$$

We can split the final component of (3.6) dependent on whether f and f' belong to the same E_i:

$$\begin{aligned}
&\{\text{res}_{x_n}(f, f') \mid f, f' \in E, f \neq f'\} \\
&\quad = \bigcup_{i=1}^{t} \{\text{res}_{x_n}(f, f') \mid f, f' \in E_i, f \neq f'\} \\
&\qquad \cup \{\text{res}_{x_n}(f, f') \mid f \in E_i, f' \in E_j, i \neq j, f \neq f'\} \\
&\quad = \bigcup_{i=1}^{t} \{\text{res}_{x_n}(f, f') \mid f, f' \in E_i, f \neq f'\} \cup \text{RES}^{\times}(\mathcal{E}).
\end{aligned}$$

Hence gathering under the union we obtain:

$$\begin{aligned}
{}_{\mathbf{M}}\mathbf{P}(E) = \bigcup_{i=1}^{t} \Big[&\bigcup_{f \in E_i} \{a_i \mid f = \sum_{i=0}^{k_f} a_i x^i, a_i \neq 0\} \\
&\cup \{\text{disc}_{x_n}(f) \mid f \in E_i\} \\
&\cup \{\text{res}_{x_n}(f, f') \mid f, f' \in E_i, f \neq f'\}\Big] \\
&\cup \text{RES}^{\times}(\mathcal{E}) \\
= \bigcup_{i=1}^{t} &{}_{\mathbf{M}}\mathbf{P}(E_i) \cup \text{RES}^{\times}(\mathcal{E}).
\end{aligned}$$

Hence we see that

$${}_{\mathbf{M}}\mathbf{P}(\mathcal{R}(\Phi)) = {}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$$

as we required.

□

We can use Theorem 3.7 to easily compute a TTICAD with existing technology, but only in the case that each quantifier-free formula φ_i contains an equational constraint and no equational constraints are nullified (otherwise the lifting stage of Algorithm 3.1 is altered).

Corollary 3.8.
If each φ_i contains an equational constraint and no f_i is nullified by a point in $\mathbb{R}^{n-1}$ then inputting $\mathcal{R}(\Phi)$ into an implementation of `CADW` *(which produces a sign-invariant CAD using McCallum's projection operator), will result in the TTICAD for Φ produced by Algorithm 3.1.*

This allows us to produce TTICADs in technologies such as QEPCAD that are simpler than a sign-invariant CAD. However the conditions on Corollary 3.8 are restrictive and Algorithms 3.1 and 3.2 can be applied to many more examples (and also include advances such as improved lifting). It would be of great use to be able to identify whether a problem is suitable for ResCAD before any construction took place, however as Corollary 3.8 depends on nullification in the lifting stage this is unlikely.

3.4.2 Semi-restricted Projection and Bi-equational Constraints

In Section 2.4.4 the equational constraint projection operator [McC99] was introduced, which was generalised to the truth-table invariant projection operator (Definition 3.4). McCallum [McC01] extended the idea of equational constraints to a semi-restricted projection operator

$$_{\mathbf{M}}\mathbf{P}^*_E(A) := {}_{\mathbf{M}}\mathbf{P}_E(A) \cup \{\text{disc}_{x_n}(g) \mid g \in A, g \notin E\}.$$

Whilst $_{\mathbf{M}}\mathbf{P}^*_E(A)$ is a superset of the equational constraint, it guarantees order-invariance of the $g \in A$ in sections of f over cells. Therefore $_{\mathbf{M}}\mathbf{P}^*_E(A)$ can be used repeatedly throughout the whole algorithm, unlike $_{\mathbf{M}}\mathbf{P}_E(A)$ which can only be applied at the highest level.

A logical extension of the projection and lifting TTICAD algorithm would be to expand the semi-restricted projection to deal with TTICAD. Including the discriminants of the non-equational constraints with $_{\mathbf{TTI}}\mathbf{P}$ would be an interesting first investigation, although from [McC01] we would only gain order invariance of each g in sections of the equational constraint of the same sub-formula as g. Whilst this seems sufficient for one projection/lifting phase whilst constructing a TTICAD, it may prove problematic when used repeatedly, and should be investigated further. Care needs to also be taken if $A \setminus E \neq \bigcup_{i=1}^{m} A_i \setminus E_i$, although the problematic polynomials are equational constraints and so order invariance is already guaranteed.

In [BM05] the authors investigate extending the theory of equational constraints to two polynomials. This results in a CAD invariant with respect to the variety $V(f_1, f_2)$ rather than a single equation. This is an extension of the fact that if f_1 and f_2 are both equational constraints, then so is their resultant. It should be profitable to look at applying this theory to TTICAD: taking advantage of sub-formulae with multiple equational constraints.

3.5 Regular Chains Algorithm

Constructing a cylindrical algebraic decomposition by regular chains technology is possible in two ways. In [CMXY09] (described in Section 2.5.2) this method of constructing CADs was introduced and proceeds by producing a complex cylindrical decomposition according to the triangular decomposition of regular chains and translating into real space by real root isolation (this process is somewhat recursive, and so we denote it RC-Rec-CAD). This can only generate a sign-invariant CAD, but RC-Rec-CAD proves competitive, and sometimes more efficient, than projection and lifting CAD implementations.

In [CM12] (described in Section 2.5.3) an alternative algorithm was presented to construct CADs through complex space and regular chains. This algorithm works by constructing the complex cylindrical decomposition incrementally by polynomial: refining an existing complex cylindrical tree whilst maintaining cylindricity. Once all polynomials have been processed the tree is converted into a CAD (and we denote this entire approach RC-Inc-CAD) This new approach is much more efficient, partly as it allows for the recycling of subresultant calculations.

One major benefit of the incremental approach over the original recursive algorithm is that all equational constraints can be utilised. When refining the complex cylindrical tree with respect to an equational constraint then any branch for which the constraint is not satisfied can be truncated. As this process can be done in any refinement step with respect to an equational constraint it allows all possible constraints to be used. This offers a distinct advantage to projection and lifting with equational constraints which usually can only utilise a single equational constraint (or, at most, two equational constraints [BM05]).

We now describe work that combines the application of equational constraints to RC-Inc-CAD with truth table invariance to build RC-Inc-TTICADs. The adaption of the RC-Inc-CAD is not trivial and requires new algorithms and implementation. The work will be published in [BCD$^+$14] and resulted from collaboration between the University of Bath research group with Marc Moreno Maza (University of Western Ontario) and Changbo Chen (CIGIT, Chinese Academy of Sciences). As the author of this thesis was involved in the discussions and experimentation of this topic, but the theory and implementation was mainly completed by other researchers on the paper, we will not go into detail of the algorithm but concentrate on its features. The full details of the theory and implementation can be found in [BCD$^+$14].

3.5.1 RC-TTICAD Algorithm

Recall that a complex cylindrical decomposition (Definition 2.38) is a partition of $\mathbb{C}^n$ such that for any pair of cells $\{C_1, C_2\}$ their canonical projections to $\mathbb{C}^k$, for $1 \leq k < n$, are equal or disjoint. Further, recall from Definition 2.40 that a **complex cylindrical tree** (**CCT**) is a rooted tree describing a cylindrical decomposition.

Assume that T is a rooted tree, with nodes at depth i of the form: "any x_i", "$p = 0$", or "$p \neq 0$" (for some $p \in \mathbb{Q}[x_1, \ldots, x_i]$). Let T_i indicate the induced subtree of depth i, and for a path Γ let the zero set, $Z_{\mathbb{C}}(\Gamma)$ be the intersection of the zero sets of its notes. Let the zero set of T, denoted $Z_{\mathbb{C}}(T)$, be the union of the zero sets of its paths.

A **complete complex cylindrical tree** (**complete CCT**) is a tree where each node either has one child ("any x_i") or has $s+1$ children defined by "$p_1 = 0$",...,"$p_s = 0$" and "$\prod_i p_i \neq 0$" (where the $p_i(\alpha, x_n)$, specialised to any $\alpha \in Z_{\mathbb{C}}(\Gamma)$ for any path Γ ending at the node, are squarefree, co-prime, and have non-vanishing leading coefficient).

Definition 3.8.
For a complete complex cylindrical tree T, we define the **complex cylindrical decomposition of $\mathbb{C}^n$ associated with** T to be the set:

$$\{Z_{\mathbb{C}}(\Gamma) \mid \Gamma \text{ is a path of } T\}.$$

Definition 3.9.
Let T be a complex cylindrical tree of $\mathbb{C}^n$ and let Γ be a path of T. A polynomial $p \in \mathbb{Q}[x_1, \ldots, x_n]$ is **(path) sign invariant on** Γ if either $Z_{\mathbb{C}}(\Gamma) \cap Z_{\mathbb{C}}(p) = \varnothing$ or $Z_{\mathbb{C}}(\Gamma) \subseteq Z_{\mathbb{C}}(p)$. A constraint $p = 0$ or $p \neq 0$ is **(path) truth invariant on** Γ if p is sign invariant on Γ. A complex system cs is **truth invariant on** Γ if the conjunction of the constraints in cs is truth-invariant on Γ, and each polynomial in cs is sign-invariant on Γ.

Constructing a Complex Cylindrical Tree

We now give a description of Algorithm 3.3 which takes a list of complex systems of $\mathbb{Q}[x_1, \ldots, x_n]$ and produces a truth-invariant complex cylindrical tree. It does so by continually refining an initial tree.

After constructing a trivial CCT (consisting of a single path through nodes "any x_i"), the `IntersectLCS` algorithm repeatedly refines T according to the input systems L.

It does this by first selecting a complex system, say cs, containing an equational

Algorithm 3.3: `TTICCD(L)`: Truth table invariant complex cylindrical decomposition algorithm.

Input : A list L of complex systems of $\mathbb{Q}[x_1, \ldots, x_n]$.
Output: A complete CCT T with each $cs \in L$ truth-invariant on each path.
1 Create the initial CCT T and let Γ be its path;
2 `IntersectLCS`(L, Γ, T);

constraint, say f. It refines the tree so that f is sign-invariant. On the branch where $f \neq 0$, the system cs is discarded and `IntersectLCS` is called recursively on the branch with the remaining input. On the branch where $f = 0$, cs is replaced by $cs \setminus \{f = 0\}$ and `IntersectLCS` is called recursively on this branch with the remaining input. If no clauses with equational constraints are present then the branch is refined to be sign-invariant with respect to all remaining polynomials (identifying sufficient cases).

We omit the details and proof of correctness of Algorithm 3.3 here, but they are given in full in [BCD$^+$14]. To offer clarity of the algorithm, we offer a worked example.

Worked Example of a Class of Problems

To illustrate the algorithm, consider a general input of two complex systems,

$$L = [cs_1, cs_2] := [\{f_1 = 0, g_1 \neq 0\}, \{f_2 = 0, g_2 \neq 0\}] .$$

We first construct the initial tree, and refine with respect to cs_1 (the first system with an equational constraint). This will refine to a sign-invariant tree for f_1 (with the two branches corresponding to the sign of f_1).

For the branch where $f_1 \neq 0$, the system cs_1 will be discarded and `IntersectLCS` will be called recursively for $[cs_2]$. This will refine to the only sufficient case where $f_2 = 0$ and $g_2 \neq 0$.

For the branch where $f_1 = 0$ we remove f_1 from cs_1 and refine according to $[\{g_1 \neq 0\}, \{f_2 = 0, g_2 \neq 0\}]$. This now identifies the constraint $f_2 = 0$ and we must distinguish between the cases $f_2 = 0$ and $f_2 \neq 0$.

For the branch where $f_2 \neq 0$ then we remove cs_2 and recursively call `IntersectLCS` with just $[\{g_1 \neq 0\}]$. This refines with respect to the sign of g_1 and identifies the only sufficient case $g_1 \neq 0$.

Finally, for the case where $f_2 = 0$ (and also $f_1 = 0$), we call `IntersectLCS` recursively with $[\{g_1 \neq 0\}, \{g_2 \neq 0\}]$. This refines with respect to the signs of $\{g_1, g_2\}$.

This process results in a case discussion that is summarised by Figure 3.7.

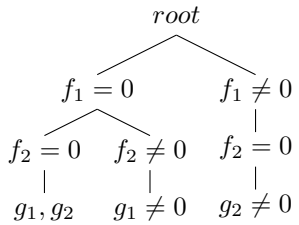


Figure 3.7: Case distinction for $L = [cs_1, cs_2]$.

Algorithm 3.4: `RC − TTICAD(L)`: Truth table invariant (reglar chains) CAD algorithm.

Input : A list L of semi-algebraic systems of $\mathbb{Q}[x_1, \ldots, x_n]$.
Output: A CAD such that each $sas \in L$ is truth-invariant on each cell.

1 Set L' to be the list of corresponding complex systems ;
2 $\mathcal{D} :=$ `TTICCD`(L') ;
3 `MakeSemiAlgebraic`$(\mathcal{D}, \mathtt{n})$

Producing a TTICAD from a TTICCD

The final step is shown in Algorithm 3.4, which gives an algorithm to construct a TTICAD with regular chains technology. It makes use of `MakeSemiAlgebraic` from [CMXY09], which takes a complex cylindrical decomposition $\mathcal{C}$ and returns a CAD $\mathcal{D}$ of $\mathbb{R}^n$ such that for each cell $C \in \mathcal{C}$ the set $C \cap \mathbb{R}^n$ is a union of cells in $\mathcal{D}$. Therefore $\mathcal{D}$ is still truth-invariant for each complex system and so is a TTICAD for the original input.

The proof of correctness for Algorithm 3.4 is given in [BCD$^+$14].

Complexity Comparison

Within [BCD$^+$14] a comparison was given between building a sign-invariant CAD incrementally with regular chains and building a TTICAD with the same technology. This was completed by one of the other authors and we summarise their results, which demonstrate the power of the new algorithms.

We consider combination diagrams such as in Figure 3.7.

Theorem 3.9 ([BCD$^+$14])**.**
Let L be a list of r complex systems. Assume each complex system of L has s equational constraints and t constraints of other types.

Then the number of constraints in a sign-invariant computational diagram is

$$2^{r(s+t)+1} - 1.$$

The number of constraints appearing in a truth table invariant computational diagram is

$$2(s + 2^t)^r - 2.$$

3.6 Implementation and Experimentation: Regular Chains TTICAD

The implementation of Algorithm 3.4 and relevant sub-algorithms was conducted by collaborators within the development `RegularChains` library. This was then loaded into the development version of MAPLE using the latest procedures (such as improved polynomial representation and real root isolation).

3.6.1 Experimental Results for TTICAD by Regular Chains

Experiments were conducted to consider the effectiveness of regular chains TTICAD compared to: other regular chains CAD algorithms; projection and lifting TTICADs and sign-invariant CADs; other state-of-the-art CAD algorithms.

A set of CAD examples were sourced from CAD papers [BH91, BDE$^+$13], system solving papers [CGL$^+$07, CM12], and generated by branch cuts of algebraic relations (detailed in Sections 2.8.1 and 3.9). For problems in the first two sets, alternative logical formulations were formed by producing disjunctions where every subformula contains an equational constraint (denoted by †) or where only some subformulae contain an equational constraint (denoted by ††).

A representative subset of the problems are given in Table 3.3. Each problem was accompanied by a variable ordering, and the number of variables is shown in the column below n. For each result the cell count and time taken (in seconds) to construct the CAD is recorded, with T/O indicating a time out (set at 30 minutes). FAIL indicates an algorithm returning a theoretical failure (for example the input not being well-oriented) whilst Err indicates an unexpected error (that appears to be a result of the implementation rather than theoretical).

We first compare RC-TTICAD with RC-Inc-CAD and RC-Rec-CAD, and PL-TTICAD and PL-CAD.

We can clearly see that RC-TTICAD never gives a higher cell count than any of the regular chains or projection and lifting algorithms. Compared to the sign-invariant CADs we see that RC-TTICAD offers a saving of at least an order of magnitude. This coincides with an, often significant, general saving in time from using RC-TTICAD. We

Problem	n	RC-TTICAD		RC-Inc-CAD		RC-Rec-CAD		PL-TTICAD		PL-CAD		Mathematica	Qepcad		SyNRAC		Redlog	
		Cells	Time	Cells	Time	Cells	Time	Cells	Time	Cells	Time	Time	Cells	Time	Cells	Time	Cells	Time
Intersection†	3	541	1.0	3723	12.0	3723	19.0	579	3.5	3723	29.5	0.1	3723	4.9	3723	12.8	Err	—
Ellipse†	5	71231	317.1	81183	544.9	81193	786.8	FAIL	—	FAIL	—	11.2	500609	275.3	Err	—	Err	—
Solotareff†	4	2849	8.8	54037	209.1	54037	539.0	FAIL	—	54037	407.6	0.1	16603	5.2	Err	—	3353	8.6
Solotareff††	4	8329	21.4	54037	226.9	54037	573.4	FAIL	—	54037	414.3	0.1	16603	5.3	Err	—	8367	13.6
2D Ex†	2	97	0.2	317	1.0	317	2.6	105	0.6	317	1.8	0.0	249	4.8	317	1.1	305	0.9
2D Ex††	2	183	0.4	317	1.1	317	2.6	183	1.1	317	1.8	0.0	317	4.6	317	1.2	293	0.9
3D Ex†	3	109	3.5	3497	63.1	3525	1165.7	109	2.9	5493	142.8	0.1	739	5.4	—	T/O	Err	—
MontesS10	7	3643	19.1	3643	28.3	3643	26.6	—	T/O	—	T/O	T/O	—	T/O	—	T/O	Err	—
Wang 93	5	507	44.4	507	49.1	507	46.9	—	T/O	T/O	—	897.1	FAIL	—	Err	—	Err	—
Rose†	3	3069	200.9	7075	498.8	7075	477.1	—	T/O	—	T/O	T/O	FAIL	—	—	T/O	Err	—
genLinSyst-3-2†	11	222821	3087.5	—	T/O	—	T/O	FAIL	—	FAIL	—	T/O	FAIL	—	Err	—	Err	—
BC-Kahan	2	55	0.2	409	2.4	409	4.9	55	0.2	409	2.4	0.1	261	4.8	409	1.5	Err	—
BC-Arcsin	2	57	0.1	225	0.9	225	1.9	57	0.2	225	0.9	0.0	225	4.8	225	0.7	161	2.4
BC-Sqrt	4	97	0.2	113	0.5	113	1.3	FAIL	—	113	0.6	0.0	105	4.7	105	0.4	73	0.0
BC-Arctan	4	211	3.5	—	T/O	—	T/O	FAIL	—	—	T/O	T/O	—	T/O	Err	—	—	T/O
BC-Arctanh	4	211	3.5	—	T/O	—	T/O	FAIL	—	—	T/O	T/O	—	T/O	Err	—	—	T/O
BC-Phisanbut-1	4	325	0.8	389	1.8	389	5.8	FAIL	—	389	3.6	0.1	377	4.8	389	2.0	217	0.2
BC-Phisanbut-4	4	543	1.6	2007	13.6	2065	21.5	FAIL	—	51763	932.5	11.9	51763	8.6	Err	—	Err	—

Table 3.3: Comparing the RC-TTICAD algorithm with other forms of CAD and implementations.

can also see explicitly that the TTICAD algorithms can take advantage of the logical structure of the formula by the difference in cell counts for † and †† problems (which is not the case for sign-invariance).

We see that sometimes constructing a TTICAD by regular chains is more efficient than by projection and lifting (although never the reverse). Further, the regular chains algorithm never returns FAIL, whilst the projection and lifting algorithm fails for precisely half the examples. We discuss in more detail in Section 3.7 the differences in the algorithms that account for this behaviour.

The implementations of QEPCAD, REDLOG and SYNRAC all are projection and lifting based. As was shown in Section 3.2.1 and Table 3.1, TTICAD theory can offer greater savings than implicit equational constraints and partial CAD techniques (as implemented in QEPCAD) when all clauses have equational constraints. This is confirmed in Table 3.3.

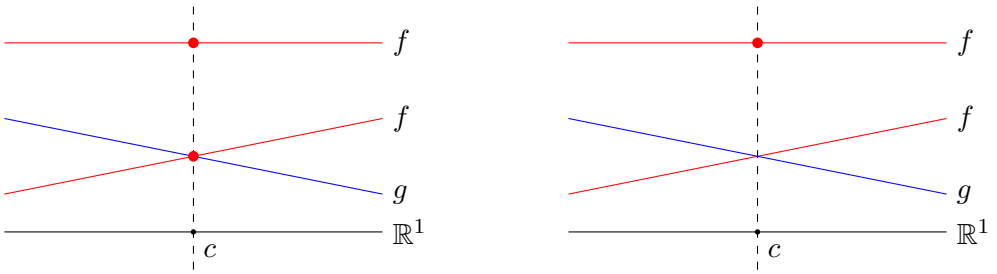
Both SYNRAC and `Redlog` fail for a large number of examples: the former returning an error message and the latter suspending during construction producing no output or error messages. When they complete computation they are often competitive as they are optimised (for example REDLOG offers partial lifting techniques). Whilst we use the most current public version of SYNRAC there is a superior development version which we do not have access too (that would presumably fail on fewer examples). REDLOG is intended for quantifier elimination by virtual substitution rather than CAD but can be forced to construct CADs.

We note that MATHEMATICA is often the quickest algorithm, and often by a significant amount. As mentioned elsewhere in this thesis, the output of MATHEMATICA is not a CAD and so a comparison is perhaps not fair, although it is worth noting that MATHEMATICA times out on 5 examples (whilst RC-TTICAD is successful for all problems).

It is clear that the results in Table 3.3 demonstrate that the RC-TTICAD is a competitive and state-of-the-art CAD algorithm.

3.7 Comparison of Projection and Lifting and Regular Chains TTICAD

We now compare the two algorithms for computing a TTICAD. It was shown in Table 3.3 that constructing a TTICAD by regular chains is often more efficient than by projection and lifting and that it avoids theoretical failure. These differences are, at least partly,



(a) Projection and Lifting TTICAD. (b) Regular Chains TTICAD.

Figure 3.8: Case distinction in TTICADs for $\varphi := [f = 0 \wedge g > 0]$.

due to the following properties of the two algorithms.

3.7.1 Case Distinction

We first note that constructing a TTICAD by regular chains allows for a finer case distinction than by projection and lifting. We demonstrate with a simple example how it can avoid constructing certain cells if the truth value of a formula is already known.

Consider a clause of the form $\varphi := [f = 0 \wedge g > 0]$ in two variables and let c be a cell in the induced CAD of $\mathbb{R}^1$ corresponding to an intersection of f and g, as shown in Figure 3.8. Even though f and g intersect within the stack over c, the truth value of φ does not change at this intersection: g is a strict inequality so φ cannot be satisfied on a 0-cell, and the cells directly above and below the intersection correspond to $f \neq 0$ so φ is also false.

Using the projection and lifting algorithm will identify all cells where $f = 0$ and so identifies the extraneous cell in the lifting phase, as shown in Figure 3.8a. The regular chains algorithm will not identify this intersection as a cell: during construction of the complex cylindrical tree it will discard the branch corresponding to this cell. It therefore only considers cells over c where $f = 0$ and $g \neq 0$, as shown in Figure 3.8b.

Whilst this only reduces the cell count by 2 cells in this case, it can obviously have a greater effect with more intersections or formulae.

3.7.2 Multiple Equational Constraints

With the introduction of the sign-invariant incremental algorithm for CAD in [CM12], every equational constraint of a problem can be utilised due to the case analysis when refining the complex cylindrical tree. This is unlike construction with the older regular chains algorithm from [CMXY09] (where no equational constraints can be used) or by

projection and lifting (where, at most, two equational constraints can be considered).

Similarly, when constructing a TTICAD incrementally using regular chains we can consider all equational constraints for each formula. This produces further savings over the projection and lifting algorithm. Whilst this initially seems to remove the problem of choosing an equational constraint to designate for use (discussed in Section 5.2.2), there is still a choice of which order to consider the equational constraints in each formula. This turns out to be an important choice and is investigated further in [EBC+14] (and discussed in Section 5.2.4).

3.7.3 Well-orientedness

One of the issues of constructing an equational constraint or truth table invariant CAD by projection and lifting is theoretical failure due to a lack of well-orientedness. If a polynomial is nullified on a cell of positive dimension, then this can lead to theorems validating the order/sign-invariance not being applicable.

When constructing a TTICAD through regular chains there is no well-orientedness condition, and any problem will complete construction of a TTICAD (given sufficient time and memory). This means we will never have theoretical failure, which makes the regular chains algorithm much more widely applicable than projection and lifting.

Comparison of the two algorithms could lead to results concerning whether well-orientedness is a necessary condition for the construction of the projection and lifting CAD in question, or if it is merely a theoretical necessity for the current theorems. Ideally, a stronger condition would be created that reduces the rate of failure for projection and lifting, or an improved projection and lifting algorithm that never results in theoretical failure.

3.7.4 Disjunctive Normal Form

There is a drawback to the implementation of Algorithm 3.4 in that the input must be given as a disjunction of systems. If a problem is not in a disjunctive form then it must first be put in a disjunctive normal form[3]. This can be expensive, with the minimal disjunctive normal form of $[A_1 \vee B_1] \wedge \cdots \wedge [A_m \vee B_m]$ requiring 2^m conjunctive formulae.

In Theorem 3.9 it was shown that in constructing the complex cylindrical tree for a problem the number of constraints considered is exponential in the number of formulae.

[3]This can be done algorithmically: MAPLE offers the `Logic[Canonicalize]` function which can be given the option `form=DNF`. Note that this does not give a minimal normal form: $[A_1 \vee B_1] \wedge [A_2 \vee B_2]$ gets converted into a disjunction of 9 formulae, each of size 4, whilst the minimal normal form is $[A_1 \wedge A_2] \vee [A_1 \wedge B_2] \vee [B_1 \wedge A_2] \vee [B_1 \wedge B_2]$.

Specifically, for r complex systems, each with s equational constraints and t constraints of other types, the truth table invariant computational diagram contains

$$2(s + 2^t)^r - 2$$

constraints. Therefore an increase in the number of these systems can prove very expensive computationally[4].

3.8 Idea for Extension: Partial TTICAD

The construction of a partial CAD (Section 2.4.2) involves using deductions on the truth value of a formula to simplify the lifting phase of constructing the CAD. We now consider how this might apply to TTICADs.

Consider a formula:

$$\Phi := [\varphi_1 \vee \cdots \vee \varphi_t],$$

and assume that each φ has a designated equational constraint $f_i = 0$.

It may be possible to adapt the partial CAD techniques to work on each individual formula. When preparing to lift over a cell, $c \in \mathcal{D}'$, from $\mathbb{R}^{n-1}$ to $\mathbb{R}^n$ then we can consider the truth value of each φ_i.

It may be possible to decide the truth of φ_i on c before lifting. For example if $\varphi_i = [f_i(x_1, \ldots, x_n) = 0 \wedge g(x_1, \ldots, x_{n-1}) > 0 \wedge \hat{\varphi}_i(x_1, \ldots, x_n)]$ and g is negative on c then the value of φ_i will be false in every cell above c. In this case then we cannot simply construct the trivial cylinder over c as other φ_j may change truth value. However, we can remove f_i from the lifting set over c.

Remark 3.2.
Removing certain f_i when lifting over a cell c of $\mathbb{R}^{n-1}$ will clearly produce fewer cells and thus improve the efficiency of the projection and lifting TTICAD algorithm. Further, if the f_i being excluded was nullified on c, violating the well-orientedness condition for the TTICAD algorithm (Definition 3.6), then this partial technique could avoid theoretical failure and expand the application of Algorithms 3.1 and 3.2.

Further, imagine that Φ is preceded by a sequence of quantifiers:

$$\Psi := (Q_{k+1}\ x_{k+1}) \cdots (Q_n\ x_n)\,[\varphi_1 \vee \cdots \vee \varphi_t],$$

[4]Further, if the disjunctive normal form is computed algorithmically in MAPLE then r will generally be larger than for the optimal normal form, and the values of s and t will likely be increased as well.

where each Q_i is a universal or existential quantifier.

If Q_n is an existential quantifier we can distribute over the disjunction:

$$\Psi \equiv (Q_{k+1}\ x_{k+1}) \cdots (Q_{n-1}\ x_{n-1})\left[[(\exists\ x_n)\varphi_1] \vee \cdots \vee [(\exists\ x_n)\varphi_t]\right].$$

Again, we may be able to decide the truth of certain $(\exists\ x_n)\varphi_i$ before finishing the lifting process: as soon as a point is found over c satisfying φ_i we can stop lifting with respect to f_i and denote φ_i as **TRUE** in the entire cylinder over c. We may also avoid theoretical failure, as mentioned in Remark 3.2.

We could extend these ideas by keeping track of when sections are produced due to a single formula. Consider lifting over c to the cells d_1, d_2, d_3 where d_2 is a section produced just from polynomials in φ_i (from $P_{E_i}(A_i)$). Then for all φ_j where $j \neq i$ then the polynomials in $P_{E_j}(A_j)$ will be delineable over $d_1 \cup d_2 \cup d_3$, therefore only a single lifting need be conducted. This is not the case for polynomials in $P_{E_i}(A_i)$ or the cross-resultants which should be lifted over d_1, d_2, and d_3 separately. This is analogous to the cluster based CAD algorithm in [Arn88] (described in Section A.4.7).

How to utilise this case distinction is not an obvious choice. The single lifting for those formulae not requiring this particular section could be merged back into the CAD, or the CAD could "branch" into multiple truth-invariant CADs for each formula, with a known relation between all the cells. The latter option seems unduly expensive, but the branching could occur only over certain cells, offering a CAD that is "exploded" at certain points, which would reduce the cost and could prove efficient (especially if by not lifting over certain sections it avoids computing with expensive algebraic numbers).

3.9 Application: Branch Cut Analysis

We discuss in greater detail an application of CAD that is particularly suited for TTI-CAD: verification of identities in the presence of branch cuts. This was initially discussed in Section 2.8.1 and the original work in this section was published in [DBEW12], [EBDW13], and [ECTB$^+$14]. The author was involved in many of the discussions for the work discussed but the majority of the work was conducted by other members of the research group.

3.9.1 Verification in the Presence of Branch Cuts

As discussed in Section 2.8.1, and covered in great detail in [Phi11], CAD can be used to decide the validity of identities over the complex plane. When considering an identity

involving elementary functions such as log, $\sqrt{\cdot}$, or inverse trigonometric functions then the geometry of the branch cuts needs to be considered to determine the regions where the identity is valid.

Verifying a complex identity can be approached with CAD, as described in Algorithm 2.5, by: determining the branch cuts; representing them as semi-algebraic equations in $\Re(z)$ and $\Im(z)$; generating a CAD of $\mathbb{R}^{2n} \equiv \mathbb{C}^n$ according to these branch cuts; evaluating the identity at each sample point (proving identical truth or generic falsity on each cell). This is unfortunately necessary as many complex identities that seem obvious are not valid for the whole plane, for example:

$$\sqrt{z-1}\sqrt{z+1} \stackrel{?}{=} \sqrt{z^2-1}. \tag{3.7}$$

Whilst (3.7) appears valid, it is only correct for complex $z \in \mathbb{C}$ such that $\Re(z) \geq 0$ or $\Im(z) = 0 \wedge \Re(z) \geq -1$.

In [DBEW12], this and other approaches to proving identities were discussed and some of their shortcomings were identified. Three key examples were discussed: the Kahan arccosh example from [Kah87]; the Joukowski conformal map; and, the arctan addition rule.

The Kahan problem involves the simplification of a conformal map from fluid dynamics involving arccosh. Whilst the branch cut for arccosh is simply the real axis between $(-\infty, 1)$ (as defined in [AS72]), this simplification transforms the cuts so that it holds over the entire complex plane, except for a small teardrop region:

$$\left\{ z = x + iy \;\middle|\; |y| \leq \sqrt{\frac{-(x+3)^2(2x+9)}{2x+5}},\ -\frac{9}{2} \leq x \leq -3 \right\}.$$

This is isolated by 7 transformed branch cuts, each described by a single equality and inequality. The arctan addition formula for two real variables, (x, y), is true when $|1 - xy| < 1$ due to a "branch cut at infinity" and is an example of real variables still being affected by branch cuts.

The discussion of the Joukowski's map:

$$f : z \mapsto \frac{1}{2}\left(z + \frac{1}{z}\right),$$

consists of trying to prove bijectivity from $D := \{z \mid |z| > 1\}$ to $\mathbb{C}^\ddagger := \mathbb{C} \setminus [-1, 1]$. The quantified formula constructed to describe this bijectivity proved too difficult to naïvely solve, which led to communications with Brown [Bro12], who maintains QEPCAD-B. In

manipulating the problem to be better suited for QEPCAD, he inspired work on how to best express problems for CAD that is discussed in Chapter 6.

3.9.2 Understanding Branch Cuts

In [EBDW13] methods of determining and describing branch cuts were given. There are two main methods of determining branch cuts: by decomposing into real variables or using a complex parametric representation. Whilst the latter can be useful for visualisation, it is noted in [EBDW13, Section 4] that the former can provide semi-algebraic output for use with CAD.

These algorithms were implemented in MAPLE 17+ within the `FunctionAdvisor` command. Given an expression in one complex variable, `FunctionAdvisor` can provide a description of the relevant branch cuts, either in two real variables or a parametrised complex variable, as well as visualisations of the branch cuts. `FunctionAdvisor` also applies simplification, removing spurious branch cuts, where possible The details of this implementation are given in [ECTB+14] and the functionality is available in versions of MAPLE from 17 onwards.

The semi-algebraic sets output from this algorithm all describe branch cuts and consist of equalities and inequalities. For example, the first set for the Kahan example is:

$$\big[8y^3x + 8yx^3 + 20y^3 + 84yx^2 + 288yx + 324y = 0,\\ -225x^2 - 324x + 63y^2 - 4x^4 - 52x^3 + 12y^2x + 4y^4 < 0\big].$$

We wish to describe the space as decomposed by these semi-algebraic sets and previously a sign-invariant CAD would need to be constructed with respect to all polynomials: producing 409 ($x \prec y$) or 1,143 ($y \prec x$) cells for the Kahan example. It is clear that a TTICAD for the sets will suffice for deciding the validity of the simplification with respect to these branch cuts and this offers a huge saving in cells: 55 ($x \prec y$) and 39 ($y \prec x$) cells for PL-TTICAD and RC-TTICAD. These cell counts are more efficient than both QEPCAD (261 and 1143 cells) and MATHEMATICA (72 and 278 cells).

In general when analysing a simplification with respect to branch cuts a TTICAD is the optimal choice of CAD. We are only concerned at interaction of polynomials in separate sets when the branch cuts intersect, which occurs when the equalities defining them are simultaneously zero (and the inequalities are also satisfied). Therefore TTICAD is more appropriate than a sign-invariant CAD (or an equational constraint CAD with

respect to the implicit equational constraint). Further, a truth-invariant CAD is not appropriate as the polynomials are not part of a larger formula.

3.10 Solotareff-3

The Solotareff-3 problem introduced in Section 2.12 is not particularly interesting for TTICAD application. The formulation given in (2.13) consists of a conjunction of four equalities and eight inequalities and so does not have the disjunctive structure that showcases the strength of truth table invariance: a TTICAD for this problem would simply be an equational constraint CAD.

We therefore give two problems derived from the Solotareff-3 problem, which we refer to as Solotareff-3† and Solotareff-3‡ in the CAD repository and experimentation in this thesis.

$$\begin{aligned}\dagger : \Big[\big[[3v^2 - 2v - a = 0] \ \wedge \ [v^3 - v^2 - av - 2b + a - 2 > 0] \ \wedge \ [1 \leq 4a] \\ \wedge \ [4a \leq 7] \ \wedge \ [-1 \leq v] \ \wedge \ [v \leq 0]\big] \ \vee \ \big[[3u^2 - 2u - a = 0] \wedge \\ [u^3 - u^2 - au - a + 2 > 0] \ \wedge \ [-3 \leq 4b] \ \wedge \ [4b \leq 3] \ \wedge \ [0 \leq u] \ \wedge \ [u \leq 1]\big]\Big]. \quad (3.8)\end{aligned}$$

$$\begin{aligned}\ddagger : \Big[\big[[3v^2 - 2v - a = 0] \ \wedge \ [v^3 - v^2 - av - 2b + a - 2 > 0] \ \wedge \ [1 \leq 4a] \\ \wedge \ [4a \leq 7] \ \wedge \ [-1 \leq v] \ \wedge \ [v \leq 0]\big] \ \vee \ \big[[3u^2 - 2u - a < 0] \wedge \\ [u^3 - u^2 - au - a + 2 > 0] \ \wedge \ [-3 \leq 4b] \ \wedge \ [4b \leq 3] \ \wedge \ [0 \leq u] \ \wedge \ [u \leq 1]\big]\Big]. \quad (3.9)\end{aligned}$$

By changing the Boolean structure of the problem, we have not affected the sign-invariant algorithms but have removed the presence of an explicit equational constraint. In † there is still an implicit equational constraint, but this is not present in ‡.

We can see some interesting results in Tables 3.4 and 3.5 from various CAD techniques from the chapter. The Boolean structure changing does not affect the size of the CADs for the sign-invariant CADs, although the number of valid cells increases in ‡.

For all the experiments, the TTICAD projection operator fails due to the well-oriented condition: this is due to $3v^2 - 2va$ being nullified on a positive dimensional cell in all cases (this is also why it cannot be used in an equational constraint CAD). However, the regular chains TTICAD algorithm is not limited by this condition and successfully constructs a CAD.

Appealing to truth table invariance results in a substantial cell saving in both variable

Technique	Solotareff-3 A†			Solotareff-3 A‡		
	Cells	(Valid)	Time	Cells	(Valid)	Time
RC-Inc-TTICAD	2849	(157)	8.454	8329	(343)	21.440
RC-Inc-CAD	54037	(1914)	208.968	54037	(4510)	226.916
PL-TTICAD	**FAIL**		—	**FAIL**		—
PL-CAD (McC)	54037		407.561	54037		414.272
QEPCAD	16603		5.238	16603		5.320

Table 3.4: Solotareff † and ‡ examples with TTICAD — variable order $a \prec b \prec v \prec u$.

Technique	Solotareff-3 B†			Solotareff-3 B‡		
	Cells	(Valid)	Time	Cells	(Valid)	Time
RC-Inc-TTICAD	7891	(479)	24.937	27855	(1131)	81.194
RC-Inc-CAD	154527	(5180)	1149.671	154527	(11322)	1184.574
PL-TTICAD	**FAIL**		—	**FAIL**		—
PL-CAD (McC)	154527		1285.656	154527		1292.400
QEPCAD	49461		6.257	49461		6.430

Table 3.5: Solotareff † and ‡ examples with TTICAD — variable order $b \prec a \prec v \prec u$.

orders for Solotareff-3†: 94.7% and 94.9% in the number of total cells, respectively, with a saving of 91.8% and 90.8% in the number of valid cells. The savings are also substantial for Solotareff-3‡: 84.6% and 82.0% in the number of total cells, respectively, with a saving of 92.4% and 90.0% in the number of valid cells. In all these cases, the truth table invariance proves more powerful than the QEPCAD technology.

3.11 Conclusion

In this chapter the new concept of truth table invariance of a CAD was introduced. Given a list of quantifier-free formulae a new projection operator was given, that identifies all intra-formula intersections and only the necessary inter-formula intersections. This can be incorporated into a new algorithm to produce a TTICAD where each formula has constant truth value on each cell. The validity of the projection operator and correctness of the algorithm was proven, but only for inputs satisfying a well-orientedness condition.

The TTICAD projection operator is a subset of the McCallum projection operator, and also of the equational constraint operator with respect to the implicit equational

constraint (if present). This relation is demonstrated by experimentation with a full implementation of the TTICAD algorithm that clearly shows an increase in efficiency. An equivalent construction under certain conditions, the ResCAD set, was given along with ideas to improve the TTICAD projection operator.

The idea of truth table invariance can be combined with the incremental regular chains CAD algorithm described in Section 2.5.3. The complex cylindrical tree is refined incrementally according to the list of complex systems (derived from the formulae). This offers some notable benefits over construction by projection lifting (a more refined case distinction, ability to utilise multiple equational constraints in each formula) and perhaps most importantly does not require any well-orientedness condition. At the moment this algorithm assumes a disjunction of the formulae but future work could extend its use. Experimentation with an implementation of this method of constructing TTICADs proved that it is highly competitive with current CAD implementations.

A possible extension of TTICAD theory by incorporating partial CAD techniques with respect to the individual formulae was suggested. An application of CAD that is particularly suited for TTICAD use was given: branch cut analysis to determine the validity of an expression (generally over the complex numbers) involving elementary functions.

Chapter 4

Cylindrical Algebraic sub-Decompositions

Often an entire CAD is unnecessary to solve a problem. This issue was slightly relieved by the introduction of partial CAD [CH91] which constructs cylinders over cells but only splits them when necessary. This is therefore still a decomposition of $\mathbb{R}^n$, albeit a simplified one.

A cylindrical algebraic sub-decomposition (sub-CAD) is introduced as a subset of cells of a CAD, and can be constructed for several purposes. Different types of sub-CADs are introduced including those containing cells of specific dimensions (layered sub-CADs) and those cells that are sections of a specific set of polynomials (variety sub-CADs). These are investigated along with their mutual interactions and applications to other CAD technologies (offering the construction of structures such as layered variety sub-TTICADs).

Author's Contribution and Publication

The work in this chapter is by the author. The theory, implementation (initially in the `LayeredCAD` package and later integrated into `ProjectionCAD`), and experimentation were all done by the author. The work was then discussed with the research group for publication (incorporating feedback from reviewers).

The majority of the work in this chapter was first presented in the Technical Report [WE13]. It was then published in [WBDE14].

4.1 Definition and Motivation

Often the application of a cylindrical algebraic decomposition does not require all the cells produced. Often it is only those cells on which a given formula is satisfied or cells of certain dimensions that are needed to obtain a solution to the question at hand. This can produce thousands of superfluous cells which are not part of the solution. This excess of output is even more pertinent if the CAD is then to be used in an application (such as adjacency) which requires computations on each cell.

This chapter focuses on the identification of subsets of cells, from an overlying CAD, that are sufficient for a given problem. Often these sets can be identified in the construction phase, which saves construction time as well as reducing the size of the output CAD.

We present the following general definition:

Definition 4.1.
Let $\mathcal{D}$ be a cylindrical algebraic decomposition of $\mathbb{R}^n$, represented as a set of cells. Then any subset $\mathcal{E} \subseteq \mathcal{D}$ is a **cylindrical algebraic sub-decomposition** (**sub-CAD**).

Let $F \subset \mathbb{Q}[x_1, \ldots, x_n]$ be a set of polynomials and let $\mathcal{D}$ be a sign-invariant CAD of F. We say that any sub-CAD $\mathcal{E}$ of $\mathcal{D}$ is a **sign-invariant sub-CAD**, and similarly define sub-CADs with other invariance conditions.

Let $\varphi(x_1, \ldots, x_n)$ be a Tarski formula for which $\mathcal{D}$ is a truth-invariant CAD (φ has constant Boolean value for each cell). Then any sub-CAD $\mathcal{E}$ of $\mathcal{D}$ which contains all those cells of $\mathcal{D}$ where φ is true is called a φ-**sufficient sub-CAD**.

Assume each cell in $\mathcal{D}$ and $\mathcal{E}$ has a cell index. Then if for every cell in $\mathcal{E}$, its index is the same in both $\mathcal{E}$ and $\mathcal{D}$, then we say $\mathcal{E}$ is an **index consistent sub-CAD** of $\mathcal{D}$.

Given a quantified formula Φ we may wish to derive an equivalent quantifier-free formula, φ. For a formula over the reals this is achieved by constructing a sign-invariant CAD for the polynomials in Φ and testing the truth of Φ at a sample point of each cell. This is sufficient to draw a conclusion for the whole cell due to sign-invariance and thus an equivalent quantifier free formula can be created from the algebraic description of the cells on which Φ is true. Such an application makes no use of the cells on which Φ is false and so a Φ-sufficient sub-CAD can be used.

Of course, for a given problem we would like the smallest possible φ-sufficient sub-CAD. It is not usually possible to pre-identify this, but we have developed techniques which restrict the output of the CAD algorithm to provide sub-CADs sufficient for certain general classes of problems. These will offer savings on any subsequent computations

on the cells (such as evaluating polynomials or formulae) and in some cases also offer substantial savings in the CAD construction itself.

The sub-CADs we construct in this chapter will be index consistent and we focus on projection and lifting constructions.

4.1.1 Cylindrical Algebraic sub-Decompositions in Literature

Before discussing new algorithms we briefly offer a survey of previous work that can be described as, or easily adapted to produce a sub-CAD. Other previous work will be discussed later in this chapter relating to new concepts.

- In [McC97], whilst trying to solve a motion planning problem in the plane described by a formula φ, the author identifies a subset of cells in the decomposition of $\mathbb{R}^1$ for which any valid cell for φ must lie over. Lifting over only these cells only gives a φ-sufficient sub-CAD (and can be done in parallel). Similar ideas are in [IYAY09].

- In [Bro13] an algorithm is presented which, given polynomials F and a point α, returns a single open cell (necessarily full-dimensional) containing α on which F is sign-invariant. The cell belongs to a CAD (although not necessarily one that could be produced by any known algorithm) and hence this is an extreme example of a sub-CAD.

- Partial CAD [CH91] (discussed in Section 2.4.2) works by avoiding the splitting of cylinders into stacks when lifting over cells where the truth value is already known. If cells over which the truth value is false were discarded (rather than constructing the trivial cylinder) then a sub-CAD sufficient to analyse the input formula would be produced.

- In [SS03] an algorithm is described which takes polynomials F and returns a CAD D and theory Θ (a theory is a set of negated equations). The CAD is sign-invariant for F for all points which satisfy Θ. Rather than a sub-CAD of $\mathbb{R}^n$ this is actually a CAD of $\mathbb{R}^n_\Theta$: all those points in $\mathbb{R}^n$ except the set of measure zero which do not satisfy Θ.

- In [Str12], an algorithm is given for solving systems over cylindrical cells described by cylindrical algebraic formulae. This allows cells produced from a CAD to be used easily in further computation, which may implicitly be used to produce either sub-CADs or CADs of a sub-space.

It seems beneficial to unify these ideas under the heading sub-CAD, which allows us to notice similarities in their approaches. We will append the ideas of **Variety sub-CADs** and **Layered sub-CADs** to this list.

4.2 Variety sub-CADs

In this section we describe a way to utilise an equational constraint to restrict the output of a CAD algorithm to generate a sub-CAD. Recall the definition of an equational constraint (Section 2.4.4):

Definition 4.2.
Let φ be a Tarski formula. An **equational constraint** is an equation, $f = 0$, logically implied by φ.

We have seen that equational constraints may be given explicitly or implicitly, and the presence of an equational constraint can be utilised both in the first projection stage by refining the projection operator (Section 2.32 based on [McC99]) and also in the final lifting stage by reducing the amount of polynomials used to construct the stacks (Remark 3.1 and implemented in [Eng13b]). If more than one equational constraint is present then further savings may be possible through the theory of bi-equational constraints [McC01, BM05]. We restrict ourselves to a single equational constraint, and if multiple equational constraints are present we assume that one has been designated.

We now present the key definition for this section, that of a variety sub-CAD.

Definition 4.3.
Let φ be a Tarski formula with equational constraint $f = 0$. A truth-invariant sub-CAD for φ consisting only of cells lying in the variety defined by $f = 0$ is a **variety sub-CAD** (**V-sub-CAD**).

The inspiration for variety sub-CADs is to combine equational constraints with the key idea in partial CAD (Section 2.4.2, [CH91]) of using the logical structure of the input formula to truncate lifting in CAD. Algorithm 4.1 combines these ideas to build variety sub-CADs in the case where all factors of the equational constraint have the main variable of the system.

Algorithm 4.1 uses various sub-algorithms. The use of `ProjOp` refers to an algorithm implementing a suitable CAD projection operator. The `CADAlgo` and `GenerateStack` respectively implement compatible algorithms for CAD construction, and stack generation over a cell with respect to the sign of given polynomials (for example Algorithms

Algorithm 4.1: `VarietySubCAD`$(\varphi, \mathtt{f}, \mathbf{x})$: Variety sub-CAD algorithm.

Input : A formula φ, a declared equational constraint $f = 0$ from φ and variables $\mathbf{x} = x_1, \ldots, x_n$. φ is in $\mathbf{x}$ and all factors of f have main variable x_n.

Output: A (truth-invariant) variety sub-CAD of $\mathbb{R}^n$ for (φ, f), or **FAIL**.

```
A ← sqfreebasis(polys(φ));
E ← sqfreebasis({f});
P ← output from applying ProjOp to (A,E) once ; // First projection stage
D' ← CADAlgo(P, [x_1, ..., x_{n-1}]) ;          // Computation of a CAD of R^{n-1}
if D' = FAIL then
    return FAIL ;                                // P is not well oriented
D ← [];
for c ∈ D' do
    S ← GenerateStack(E, c);                     // Final lifting stage
    if S = FAIL then
        return FAIL ;                            // Input is not well oriented
    if |S| > 1 then
        for i = 1 ... (|S| − 1)/2 do
            D.append(S[2i]) ;                    // Cells with even index included
return D;
```

2.4 and 2.2). By compatible we mean using the same projection operator and checking for any necessary conditions of its use. This is required as some CAD algorithms may return **FAIL** if the input does not satisfy certain conditions, in which case Algorithm 4.1 must also return **FAIL**.

Algorithm 4.1 has been implemented in `ProjectionCAD`, with further details in Section C.2.

We prove that Algorithm 4.1 satisfies its specifications when the sub-algorithms used are those for equational constraints.

Theorem 4.1.

When the sub-algorithms are chosen to implement McCallum's algorithm to produce CADs with respect to an equational constraint [McC99], then Algorithm 4.1 satisfies its specification, with the produced sub-CAD consisting of cells on which the input formula has constant truth value.

Proof.

Projecting with respect to an equational constraint applies the projection operator

${}_{\mathbf{M}}\mathbf{P}_E(A)$ at the top level, then ${}_{\mathbf{M}}\mathbf{P}$ to construct the rest of the projection set. The algorithm then incrementally constructs CADs of increasing real dimension, checking for well-orientedness when building each stack. In [McC99] the author proved that the CAD returned was truth-invariant for the equational constraint and sign-invariant for any other polynomials involved on cells where the equational constraint was satisfied.

The first difference in Algorithm 4.1 is in step 9 where the final lift is performed with respect to E rather than A. This improvement follows directly from Theorem 3.2 (given in [McC99]), although it was not realised until [BDE+13, BDE+14] and was discussed in Remark 3.1. This reduces the size of the output, but not its invariance structure or correctness.

In the final loop, only some of the cells generated in the final lift are included in the output. The cells in question are a subset of what would have been produced otherwise and thus certainly a sub-CAD with the same invariance property as the complete CAD. It remains to prove that they are a variety sub-CAD (in which case we can conclude φ has constant truth value on each cell).

The only cells retained for the output are those with even index (the sections). If the polynomial f is not identically zero over a cell in $\mathcal{D}$ then these must together define its variety. If any of the polynomials in E were nullified then part of the variety may be in the sectors, but in this case the input would have failed the well-orientedness condition in [McC99] (Definition 2.26) and thus Algorithm 4.1 would return **FAIL**.

□

Remark 4.1.
As the operator, ${}_{\mathbf{M}}\mathbf{P}$, from [McC99] can return **FAIL** in situations where others do not, we consider how Algorithm 4.1 may be adapted to use alternative CAD projection operators.

First, if a polynomial in E is nullified on a cell of $\mathcal{D}$ then [McC99] returns **FAIL** while McCallum's operator to produce sign-invariant CADs in [McC98] is still applicable (because then the nullification is in the final lift where only sign-invariance and not order invariance is required). However, we cannot simply apply Algorithm 4.1 with the alternative projection operator as it will now be the case that some of the variety is contained in the sectors over the cell in question. In this case we would need the `GenerateStack` algorithm to check for nullification of E, and then if it occurs have Algorithm 4.1 include all cells from that stack in the output.

Second, if some other polynomial is nullified causing failure then ${}_{\mathbf{C}}\mathbf{P}$ and ${}_{\mathbf{CH}}\mathbf{P}$ are still applicable. As with the previous case we must still check for nullification over a cell

in the final lift, including the whole stack when nullification occurs.

In these cases there would still be output savings from building a variety sub-CAD since the inclusion of the full stack only needs to happen over those cells where nullification occurs.

We can see the strength of using a variety sub-CAD through a simple example.

Example 4.1.
Consider the simple task of describing the unit sphere: $x^2 + y^2 + z^2 = 1$ in $\mathbb{R}^3$ (with the ordering $x \prec y \prec z$). We can use a standard CAD algorithm, such as projection and lifting with respect to McCallum's projection operator, and obtain 25 cells which decomposes the whole of $\mathbb{R}^3$. However, if we only need the cells on the sphere, then we can construct a variety sub-CAD that contains the following six cells:

$$[x = -1, y = 0, z = 0],$$
$$[-1 < x < 1, y = -\sqrt{-x^2 + 1}, z = 0],$$
$$[-1 < x < 1, -\sqrt{-x^2 + 1} < y < \sqrt{-x^2 + 1}, z = -\sqrt{-y^2 - x^2 + 1}],$$
$$[-1 < x < 1, -\sqrt{-x^2 + 1} < y < \sqrt{-x^2 + 1}, z = \sqrt{-y^2 - x^2 + 1}],$$
$$[-1 < x < 1, y = \sqrt{-x^2 + 1}, z = 0],$$
$$[x = 1, y = 0, z = 0]$$

Now consider the slightly more involved question of finding regions where the following expression holds:

$$x^2 + y^2 + z^2 = 1 \wedge x + y + z - 1 > 0.$$

We can, as above, construct a CAD of the entirety of $\mathbb{R}^3$, which produces 211 cells. Alternatively, we can project with respect to the equational constraint projection operator to get the following two polynomials in $\{x, y\}$: $[y^2 + x^2 - 1, y^2 + yx + x^2 - y - x]$. Constructing a two-dimensional CAD with respect to these polynomials generates 45 cells.

If we were to proceed by the regular theory of equational constraints we would lift over all 45 cells with respect to the equational constraint defining the sphere. This produces 137 cells, but lifting onto a variety sub-CAD by Algorithm 4.1 reduces this number to 46.

We will revisit variations of this example to demonstrate other sub-CADs.

We will see later in Section 4.6.2 that for complicated examples the savings offered by using a variety sub-CAD can be substantial. Using Algorithm 4.1 clearly reduces the output size of CAD but it will save little CAD computation time since most of the work required to define the discarded cells (such as root isolation) had to be performed. There will however, be a large saving in applications which require computation on the cells of the sub-CAD.

In Algorithm 4.1 we require that the equational constraint defining the variety has factors which each have main variable x_n. This is to ensure that the lift to the variety is done at the final stage. If a formula has an equational constraint with factors not in x_n (that is, parts of the corresponding variety have lower dimension) then building a V-sub-CAD would mean even more potential cell savings, but there would also be savings in computation time since some stacks, lying off the variety, would never be built at all.

Suppose each factor of the equational constraint has main variable x_k where $k < n$. To adapt Algorithm 4.1 we must perform the restriction when lifting to a CAD of $\mathbb{R}^k$, instead of $\mathbb{R}^n$. Thus we would first build a CAD of $\mathbb{R}^{k-1}$, then perform the restricted lifting to a sub-CAD of $\mathbb{R}^k$, and continue lifting to a sub-CAD of $\mathbb{R}^n$. However, verifying this approach is a little more subtle. We cannot follow Theorem 4.1 and use McCallum's reduced projection at the first step (as the set E is considered empty according to [McC99]). If we were to use McCallum's equational constraint theory to build a variety sub-CAD of $\mathbb{R}^k$ then we would need to take care in how we lift over it (ensuring the projection polynomials above are delineable).

There are two ways to tackle these subtleties:

(a) Use the tools of McCallum's sign-invariant algorithm from [McC98] (without utilising the equational constraint) throughout. In particular, we must perform the restricted lifting with respect to the full set of projection polynomials of main variable x_k rather than just those defining the equational constraint. This is because to continue lifting with respect to projection polynomials provided by McCallum's operators we need to conclude that the sub-CAD of $\mathbb{R}^k$ is order invariant on the cells, not just sign-invariant. Thus the output sub-CAD is not a variety sub-CAD but a superset of cells containing one. Algorithm 4.2 demonstrates this approach.

(b) Use Collins-Hong projection for the first $(n-k)$ projection stages. Then apply Algorithm 4.1 with McCallum's reduced projection operator for equational constraints to build a variety sub-CAD of $\mathbb{R}^k$ (as verified by Theorem 4.1) before continuing lifting to a variety sub-CAD of $\mathbb{R}^n$.

The latter approach is still a variety sub-CAD and allows for a smaller CAD of $\mathbb{R}^k$ but these benefits may be overshadowed in the final sub-CAD of $\mathbb{R}^n$ due to lifting with respect to a larger set of polynomial in the later stages. Of course both cases may return **FAIL** in which case having all sub-algorithms implement the less efficient Collins-Hong projection operator (which never returns **FAIL**) would be a potential solution. It is worth noting that when the equational constraint is not in the main variable we may actually avoid unnecessary failure: if the input is not well-oriented but the problematic nullification only occurs on cells that are not on the variety then the outputted sub-CAD will still be valid. It is interesting to note that this sub-CAD is now a subset of a CAD we do not know how to produce algorithmically.

To allow factors of the equational constraint with different main variables would require a further extension to perform multiple stages of restricted lifting (lines $9-22$ of Algorithm 4.2) when lifting to $\mathbb{R}^i$ where x_i is a main variable of a factor, and full lifting (lines $23-29$) otherwise.

Finally, note that we have only discussed using a single (designated) equational constraint. In the case of two or more (as in $f_1 = 0 \wedge f_2 = 0 \wedge \hat{\varphi}$) we could use the theory of bi-equational constraints [McC01, BM05]. Its interaction with variety sub-CADs has not be investigated yet and would be worthwhile future work. In Section 4.4 there will also be discussion of the interaction of TTICAD (from Chapter 3) with variety sub-CADs.

4.3 Layered sub-CADs

In this section we discuss a generalisation of work from [McC93, Str00, Bro13]. The idea of returning CAD cells of full dimension (also called **open cells**) was first discussed in [McC93] and revisited in [Str00, Bro13]. All these papers discuss methods of returning only CAD cells of full-dimension, noting that this is sufficient to solve problems involving only strict polynomial inequalities. In particular, we will directly extend the CADMD algorithm from [McC93] to return cells with dimensions greater than a specified value.

We give the key definition for this section, that of a layered sub-CAD.

Definition 4.4.
Define the set of cells in a CAD of a given dimension as a **layer**. Let ℓ be an integer with $1 \leq \ell \leq n+1$. Then an **ℓ-layered sub-CAD** (**ℓ-L-sub-CAD**) is the subset of a CAD of dimension n consisting of all cells of dimension $n-i$ for $0 \leq i < \ell$. We refer to a CAD consisting of all cells of all dimensions as a **complete CAD**.

Algorithm 4.2: `VarietySubCAD`$(\varphi, f, \mathbf{x})$: Algorithm to produce sub-CADs with respect to a variety of lower dimension. This uses McCallum's projection operator (without equational constraints) throughout, and does not return a variety sub-CAD as defined in Definition 4.3, but rather a superset of one.

Input : A formula φ, a declared equational constraint $f = 0$ from φ and variables $\mathbf{x} = x_1, \ldots, x_n$. φ is in $\mathbf{x}$ and all factors of f have the same main variable.

Output: A sub-CAD $\mathcal{D}$ on which φ is truth invariant and which is the superset of a variety sub-CAD for (φ, f), or **FAIL**.

$A \leftarrow$ `sqfreebasis`(polys(φ));
$k \leftarrow \text{rank}(f)$; `// Index of` mvar(f)
Perform the first $n - k$ projection stages using `ProjOp` and starting with A;
Set $\mathbf{P_1}$ to be the projection polynomials with main variable x_i;
if $k \neq 1$ **then**
    $\mathcal{D}_{k-1} \leftarrow$ `CADAlgo`$(\mathbf{P_{k-1}}, [x_1, \ldots, x_{k-1}])$; `// Computation of a CAD of` $\mathbb{R}^{k-1}$
if $\mathcal{D}_{k-1}$ = **FAIL then**
    return FAIL ; `//` $\mathbf{P_{k-1}}$ `is not well oriented`
$\mathcal{D}_k \leftarrow []$;
if $k = 1$ **then**
    Set S to be the CAD formed by decomposing $\mathbb{R}$ according to the roots of $\mathbf{P_1}$.;
    if $|S| > 1$ **then**
        for $i = 1 \ldots (|S| - 1)/2$ **do**
            $\mathcal{D}_k$.`append`$(S[2i])$; `// Cells with even index included`
else
    for $c \in \mathcal{D}_{k-1}$ **do**
        $S \leftarrow$ `GenerateStack`$(\mathbf{P_k}, c)$; `//` k`th lifting stage`
        if S = **FAIL then**
            return FAIL ; `//` $\mathbf{P_k}$ `is not well oriented`
        if $|S| > 1$ **then**
            for $i = 1 \ldots (|S| - 1)/2$ **do**
                $\mathcal{D}_k$.`append`$(S[2i])$; `// Cells with even index included`
for $i = k + 1, \ldots n$ **do**
    $\mathcal{D}_i \leftarrow []$;
    for $c \in \mathcal{D}_{i-1}$ **do**
        $S \leftarrow$ `GenerateStack`$(\mathbf{P_i}, c)$; `//` i`th lifting stage`
        if S = **FAIL then**
            return FAIL ; `//` $\mathbf{P_i}$ `is not well oriented`
        $\mathcal{D}_i$.`append`(S) ; `// All cells included`
return $\mathcal{D}_n$;

Remark 4.2.
An ℓ-layered sub-CAD consists of the top ℓ layers of cells of a CAD. The dimensions of these cells will depend on the dimension of the space the CAD decomposes. There is an alternative description defining layered sub-CADs with respect to the minimal dimension of a cell in the sub-CAD. The convention of Definition 4.4 was chosen to make combining layered sub-CADs with other concepts, such as variety sub-CADs (Definition 4.3) more intuitive. This will be discussed in Section 4.4.

Remark 4.3.
In the literature the set of cells of full-dimensional has been referred to as an open CAD, a full CAD and a generic CAD. We prefer layered CAD as it is less open to misinterpretation and allows us to generalise the idea beyond the top dimension. The set of cells of full dimension is then a 1-layered sub-CAD and a complete CAD of $\mathbb{R}^n$ is an $(n+1)$-layered sub-CAD.

Remark 4.4.
When building a 1-layered sub-CAD it was pointed out in [Str00] that a simplified projection operator could be used. Instead of taking the full set of coefficients for a polynomial only the leading coefficient is required (since the others are there to ensure delineability if the first vanishes, but this could only happen on a cell of less than full dimension). We focus on improvements to the lifting phase, but if only a 1-layered CAD is required then this further saving in the projection phase is available. It would be interesting to investigate if this simplification can be extended further to offer a smaller projection operator for any ℓ-layered sub-CAD.

4.3.1 Direct Layered sub-CADs

In Algorithm 4.3 we describe a method to construct an ℓ-layered sub-CAD. The key step is during the lifting process, where a cell's dimension is checked during stack construction. A cell cannot increase in dimension greater than the number of lifting steps remaining and so cell's with too low a dimension can be identified and discarded. Algorithm 4.1 can be used with any valid projection operator and accompanying stack generation procedure. In particular, using Collins' projection operator with $\ell = 1$ produces the CADMD algorithm from [McC93].

Algorithm 4.3 has been implemented in `ProjectionCAD`, with further details in Section C.2. We prove that Algorithm 4.3 is valid.

Algorithm 4.3: `LayeredSubCAD`$(\varphi, \ell, \mathbf{x})$: ℓ-layered sub-CAD algorithm.

Input : A formula φ, an integer $1 \leq \ell \leq n+1$ and variables $\mathbf{x} = x_1, \ldots x_n$. φ is in $\mathbf{x}$.

Output: An ℓ-layered sub-CAD for φ, or **FAIL**.

```
1  P ← output from applying ProjOp repeatedly to φ ; // Full projection phase
2  for i = 1, ..., n do
3  |  Set P[i] to be the projection polynomials with mvar(x_i);
4  Set D[1] to be the CAD of R^1 obtained by isolating the roots of P[1];
5  for i = 2, ..., n do
6  |  D[i] ← [ ];
7  |  for c ∈ D[i − 1] do
8  |  |  dim ← Σ_{α∈c.index} (α mod 2) ;        // Lift over suitable dim cells
9  |  |  if dim > i − ℓ − 1 then
10 |  |  |  S ← GenerateStack(P[i], c);
11 |  |  |  if S =FAIL then
12 |  |  |  |  return FAIL ;                    // Input is not well oriented
13 |  |  |  else
14 |  |  |  |  D[i].append(S)
15 D ← [ ];
16 for c ∈ D[n] do
17 |  dim ← Σ_{α∈c.index} (α mod 2);
18 |  if dim > n − ℓ then
19 |  |  D.append(c);    // Remove cells of low dimension from final lift
20 return D;
```

Theorem 4.2.

Algorithm 4.3 satisfies its specification (producing an ℓ-layered sub-CAD for φ) or returns **FAIL**.

Proof.

The output being a set of cells from a valid CAD follows immediately from the correctness and compatibility of the sub-algorithms used. All cells are semi-algebraic sets and cylindrical with respect to each other. We need therefore only show that the cells in the sub-CAD produced form the top ℓ layers of the CAD.

Consider a cell, c, of dimension d in a sub-CAD of $\mathbb{R}^i$. Whilst lifting over c, it can contribute cells in the sub-CAD of $\mathbb{R}^n$ of dimension at most $d + n - i$ (as it can gain at most one dimension in each stack generation step). If cells are required for an ℓ-layered sub-CAD then they must have dimension at least $n - \ell$. Therefore we can discard c if

$d \leq i - \ell - 1$ (line 9).

When performing the final lift we must only build stacks over cells of dimension $n-\ell-1$ or greater, but the sections in those stacks will not have dimension $n-\ell$. Hence we check for this at the end (line 18) only keeping those of the required dimension.

□

Example 4.2.
Consider again the unit sphere from Example 4.1. A complete CAD contains 25 cells, and it is simple to compute: a 1-layered sub-CAD with 7 cells; a 2-layered sub-CAD with 17 cells; and a 3-layered sub-CAD with 23 cells (missing the two 0-cells $(0, 0, -1)$ and $(0, 0, 1)$) .

If we also include the plane $x + y + z - 1$ we can construct a complete CAD with 211 cells. Using Algorithm 4.3 we can construct: a 1-layered sub-CAD with 44 cells; a 2-layered sub-CAD with 135 cells; and a 3-layered sub-CAD with 197 cells.

When a problem consists of only strict inequalities, the cells describing the solutions must have full-dimension [McC93, Str00]. More generally there are classes of problems with known solution dimension. In these cases a layered sub-CAD technology will be beneficial. To give an example, consider the cyclic polynomials:

Example 4.3.
Define the **cyclic-n polynomials** to be the set of n polynomials in n variables:

$$\begin{aligned} x_1 + x_2 + \cdots + x_n &= 0, \\ x_1x_2 + x_2x_3 + \cdots + x_{n-1}x_n + x_nx_1 &= 0, \\ &\vdots \\ x_1x_2\cdots x_{n-1} + x_2x_3\cdots x_n + \cdots + x_nx_1\cdots x_{n-2} &= 0, \\ x_1x_2\cdots x_n - 1 &= 0. \end{aligned}$$

The cyclic-4 polynomials will also be used as a motivating example for the work of Chapter 6 in Example 6.1.

In [Bac89] it is shown that if there exists an integer $m > 0$ such that $m^2|n$, then there are an infinite number of solutions to the cyclic-n polynomials. Further, the solutions have dimension at least $m-1$. Therefore a layered sub-CAD containing cells of dimension $(m - 1)$ and higher would be sufficient to find the largest families of solutions.

Layered sub-CADs will also be useful when, although a sub-CAD may not be φ-sufficient, the application for the sub-CAD only requires general families of solutions.

For example, if we apply CAD to robot motion planning (discussed in detail in Chapter 6) we need only identify paths through cells of full-dimension, and so it seems a 1-layered sub-CAD may be enough. In the example considered in Chapter 6 there is an equational constraint present and so we need the full-dimensional cells on its variety, which are part of the 2-layered sub-CAD. Even further, to analyse the adjacency of such paths we may need the cells of dimension one lower and thus the cells on the variety in a 3-layered CAD will be the appropriate choice. Such a sub-CAD can be constructed by combining the ideas of variety and layered sub-CADs, which will be discussed in Section 4.4.

This example highlights that it is not necessarily obvious how many layers are needed for a sub-CAD when first considering a problem. This prompts an adaptation of Algorithm 4.3 to a recursive procedure.

4.3.2 Recursive Layered sub-CADs

When we construct a layered sub-CAD with Algorithm 4.3 we stop lifting over a cell if it cannot lead to cells of sufficient dimension in $\mathbb{R}^n$. This only happens when the cell in question is produced as a section (constructing a sector increases the dimension of a cell in a stack, unlike a section). Let us refer to such a cell as a **terminating section**. To construct a layered sub-CAD recursively (with respect to the number of layers, rather than the number of variables) we will store these terminating sections in a separate output variable, rather than discarding them. This will allow them to be used later if another layer is required.

Consider constructing a 1-layered sub-CAD, $\mathcal{D}$, and let c be a terminating section. If c is being constructed in $\mathbb{R}^i$ then the dimension of c must be $i-1$ (that is, c has co-dimension 1 within $\mathbb{R}^i$). Suppose we now wish to extend this 1-layered sub-CAD into a 2-layered sub-CAD by use of the terminating sections, which we denote $\mathcal{C}$.

If a terminating section $c \in \mathcal{C}$ is part of $\mathbb{R}^n$ then it will have dimension $n-1$ and so can be included in the 2-layered sub-CAD. Otherwise, c has co-dimension 1 in $\mathbb{R}^i$ and we can construct successive stacks over it retaining all sectors and storing sections into a new set of terminating sections. The sectors produced will be $n-1$ dimensional cells and these can be combined with the 1-layered sub-CAD to produce a 2-layered sub-CAD. The new terminating sections can then be used to produce a 3-layered sub-CAD, and we can proceed recursively in this manner. This is particularly useful if the number of layers needed is not known in advance of computation. This method is described in Algorithm 4.4.

Algorithm 4.4 has been implemented in `ProjectionCAD`, with further details in Sec-

Algorithm 4.4: `LayeredSubCADRecursive`$(\varphi, \mathbf{x}, \mathcal{C}, \mathcal{LD})$: Recursive layered sub-CAD algorithm (to produce sub-CADs with increasing numbers of layers).

Input : A formula φ, variables $\mathbf{x} = x_1, \ldots, x_n$, a list of cells of $\mathbb{R}^n$ labelled $\mathcal{LD}$, and a list of lists of cells, $\mathcal{C}$ (ordered by increasing dimension). The formula φ is in $\mathbf{x}$. The lists $\mathcal{C}$ and $\mathcal{LD}$ may be empty. Otherwise the list $\mathcal{LD}$ must contain a layered sub-CAD for φ and $\mathcal{C}$ the corresponding terminating sections.

Output: Either **FAIL** or a layered sub-CAD $\mathcal{D}'$ for φ. If $\mathcal{LD}$ was empty then $\mathcal{D}$ is a 1-layered sub-CAD and otherwise it is a layered sub-CAD with including cells of dimension one layer lower than $\mathcal{LD}$. Also, an updated list of lists of cells containing the terminating sections sufficient to construct the complete CAD.

```
1  global P ;                          // To avoid recomputing projection polynomials
2  if P is undefined then
3      P ← output from applying ProjOp repeatedly to φ ;     // Full projection phase
4      for i = 1, ..., n do
5          Set P[i] to be the projection polynomials with mvar(x_i);
6  C' ← [ ];
7  if C = ∅ then
8      D ← [ ] ;                                              // Base case - construct ℝ^1
9      Set Base to be the CAD of ℝ^1 obtained by isolating the roots of P[1];
10     for i = 1, ..., length(Base) do
11         if (i mod 2) == 1 then
12             D[1].append(Base[i]) ;     // Sectors only (odd index) for the 1-LCAD
13         else
14             C'[1].append(Base[i]) ;              // Sections (even index) so store
15     D' ← [ ];
16 else
17     D ← C ;                        // Use previously computed terminating sections
18     D' ← C[n];
19 for i = 2, ..., n do
20     for c ∈ D[i − 1] do
21         S ← GenerateStack(P[i], c);
22         if S = FAIL then
23             return FAIL ;                          // Input is not well oriented
24         for j = 1, ..., length(S) do
25             if (j mod 2) == 1 then
26                 D[i].append(S[j]) ;     // Sector (odd index) so add to output CAD
27             else
28                 C'[i].append(S[j]) ;              // Section (even index) so store
29 D' ← D' ∪ LD ;              // Combine new cells with those previously computed
30 return [D', C'];
```

tion C.2.

We prove that Algorithm 4.4 is valid.

Theorem 4.3.

Algorithm 4.4 satisfies its specification and produces a layered sub-CAD and list of terminating sections, or alternatively **FAIL**.

Proof.

As with Theorem 4.2 the proof of the correctness of Algorithm 4.4 mainly follows from the specification of the sub-algorithms used. It remains to show that the correct layers are produced.

If no terminating sections are provided, then a CAD of the real line is produced and the sectors are separated to be lifted over and Algorithm 4.4 emulates Algorithm 4.3. Otherwise, the terminating sections are used to lift over. At each stage of lifting, the sectors are retained and any sections produced are placed in $\mathcal{C}'$. All sectors produced will have co-dimension one greater than in the previous layered CAD and these sectors, together with the previous layered sub-CAD $\mathcal{LD}$, form a layered sub-CAD, $\mathcal{D}'$, with one extra layer. The new terminating sections are returned in $\mathcal{C}'$ and all have co-dimension one greater than the newly added cells of $\mathcal{D}'$.

□

Implementing Algorithm 4.4 in `ProjectionCAD` is not quite as simple as Algorithm 4.3. A global variable is used to avoid recalculation of projection polynomials (which can be costly if many resultants and discriminants are computed). Rather than outputting the terminating sections directly, as indicated in Algorithm 4.4, the implementation gives the output in two parts: the first part is the layered sub-CAD as produced, the second part is an unevaluated recursive call. This recursive call is rendered inert with Maple's unevaluated function call syntax (prefixing the command with %) which allows it to be assigned to a variable and later evaluated with the `value` command to produce a layered sub-CAD with one further layer (along with another inert recursive call). More details are given in Section C.2.

4.3.3 Order Invariance of Layered sub-CADs

We discuss an interesting property of layered sub-CADs with respect to order-invariance. We require the following lemma.

Lemma 4.4.

Let $f \in \mathbb{R}[x_1, \ldots, x_n]$ vanish identically on a cell, D, of dimension n. Then f is

identically zero on the whole of $\mathbb{R}^n$.

Proof.
We proceed by induction.

Let $n = 1$, and $D \subset \mathbb{R}^1$ an interval. As f vanishes on the whole of D, there exists at least $\deg(f) + 1$ points α_i such that $f(\alpha_i) = 0$ (there are infinitely many such points). Then by the Fundamental Theorem of Algebra, f must be the zero polynomial.

Now let $n > 1$. We view f as a univariate polynomial in x_n with coefficients in $\mathbb{R}[x_1, \ldots, x_{n-1}]$. As D is an n-dimensional cell, it must be in the cylinder of an $n-1$-dimensional cell D' in $\mathbb{R}^{n-1}$. Using the Fundamental Theorem of Algebra we can see that for every point $\alpha' \in D'$ every coefficient in f vanishes. But by induction, these coefficients must be zero on the whole of $\mathbb{R}^{n-1}$ and so $f \equiv 0$ on all of $\mathbb{R}^n$.

□

We can use Lemma 4.4 to show that 1-layered and 2-layered sub-CADs are order invariant.

Theorem 4.5.
Let $F \subset \mathbb{Z}[x_1, \ldots, x_n]$ *and* $\mathcal{D}$ *be a 1-layered or 2-layered sub-CAD of* $\mathbb{R}^n$ *sign-invariant for* F. *Then* $\mathcal{D}$ *is order-invariant with respect to* F, *meaning each polynomial has constant order of vanishing on each cell.*

Proof.
Let us first show that a 1-layered sign-invariant sub-CAD is order-invariant. This is straightforward for if a non-zero polynomial $f \in F$ is to have a non-zero order on a cell it must vanish in that cell and, as $\mathcal{D}$ is sign invariant with respect to F, it must vanish identically on that cell. For a cell $D \in \mathcal{D}$ this means that f vanishes identically on a cell of dimension n and so, by Lemma 4.4, f is the zero polynomial.

Applying this result in the 2-layered case we see immediately that each $f \in F$ is order-invariant on all n-dimensional cells in $\mathcal{D}$. Now let D' be an $(n-1)$-dimensional cell, let x_i be the dimension for which it is deficient and assume $f \equiv 0$ on the whole of D', but not identically zero on $\mathbb{R}^n$. We will show that f cannot be identically zero, and therefore its order is trivially zero. View f as univariate in x_i and factor into its content and primitive part: $\text{cont}_{x_i}(f) \cdot \text{prim}_{x_i}(f)$. Then if $f \equiv 0$ on D' then $\text{cont}_{x_i}(f)$ must be identically zero on D' (as $\text{prim}_{x_i}(f)$ can only be zero at a finite set of points). But $\text{cont}_{x_i}(f)$ is a polynomial in $n-1$ variables that vanishes on an $(n-1)$-dimensional cell and so, by Lemma 4.4, it must be identically zero on $\mathbb{R}^{(n-1)}$. Therefore $f \equiv 0$ on $\mathbb{R}^n$

and we have the desired contradiction.

□

Order-invariance is a stronger property than sign-invariance, but the extra knowledge it gives allows for the validated use of smaller projection operators (such as McCallum's projection operator in Definition 2.24). Hence this property allows for the avoidance of well-orientedness checks during stack generation when building 1 or 2-layered sub-CADs. This means not just a saving in computation time but the avoidance of unnecessary failure declarations that can sometimes follow from such checks.

4.4 Combining sub-CAD Ideas

We have discussed two types of sub-CAD in this chapter: variety and layered sub-CADs. They both can offer significant savings in cell count and time, but can also be combined to create layered variety sub-CADs, which are discussed in Section 4.4.1. It is also possible to use the idea of sub-CADs with truth table invariance (as introduced in Chapter 3) to create a wider range of sub-CADs. These are discussed in Section 4.4.2.

4.4.1 Layered Variety sub-CADs

When constructing a sub-CAD of any type, we are filtering out those cells that are relevant to the problem at hand. Constructing a variety sub-CAD does this in a single step of the lifting phase (according to an equational constraint), whilst a layered sub-CAD stratifies the cells throughout the whole lifting process (according to the dimensions of the cells). These are quite different procedures.

There is no conceptual or theoretical reason why these ideas cannot be combined to offer the benefit of both types of sub-CAD. We restrict our discussion to the case of problems with an equational constraint such that all factors of this constraint have main variable x_n and are not nullified on a lower-dimensional cell, and construct the following definition (analogous to the well-orientedness conditions of Definition 2.26 and 3.6).

Definition 4.5.
Let A be a set of n-variate integral polynomials, where $n \geq 1$, and let $E \subseteq A$ be the set of factors of an equational constraint f, which all have main variable x_n. Let $\mathcal{D}'$ be a CAD or sub-CAD of $\mathbb{R}^{n-1}$. We say that (A, E) (or the formula φ they are constructed from) are **(LV)-well-oriented** with respect to $\mathcal{D}'$ if no element of E is nullified on a cell of $\mathcal{D}'$.

This is a relatively restrictive definition and layered variety sub-CADs could be constructed for problems which do not satisfy this definition. However, to deal with other cases would require an awful lot of care and case discussion, similar to the discussion of extending the variety sub-CAD algorithms in Section 4.2.

To ensure we can keep track of the dimension of cells in a layered variety sub-CAD we require the following result.

Lemma 4.6.
Let $\mathcal{D}'$ be a sub-CAD or CAD of $\mathbb{R}^{n-1}$ for some formula φ and let c be a cell in $\mathcal{D}'$ of dimension k. Further, suppose φ is LV-well-oriented: if $f = 0$ is the equational constraint of φ then each factor of f has main variable x_n and f is not nullified on c.

Then any section of the stack lifted over c with respect to f will have dimension k.

Proof.
The proof is a straightforward application of the fact that a section of a stack has the same dimension of the cell being lifted over. Note that the condition of no nullification on c is necessary to ensure that a section of f exists, else a degenerate stack is created with no sections.

□

Lemma 4.6 shows that if we lift over a cell onto a variety with a LV-well-oriented equational constraint we will obtain cells with the same dimension. Therefore if we lift over an ℓ-layered sub-CAD of $\mathbb{R}^{n-1}$ (which contains cells of dimension $n-\ell, \dots, n-1$) we will produce a sub-CAD containing precisely those cells of dimension $n-\ell, \dots, n-1$ that lie on the variety. We formalise this idea in the following definition.

Definition 4.6.
Let φ be a Tarski formula with equational constraint $f = 0$ which has main variable x_n in all its factors, and let $1 \leq \ell \leq n$. A truth-invariant sub-CAD for φ whose cells have dimension $n - i - 1$ for $0 \leq i < \ell$ and rest on the variety defined by $f = 0$ is an **ℓ-layered variety sub-CAD** (**ℓ-LV-sub-CAD**).

Remark 4.5.
In general, an ℓ-layered variety sub-CAD consists of the top ℓ layers of cells on the variety. This can be thought of as the intersection of an $(\ell+1)$-layered CAD of $\mathbb{R}^n$ with the variety (as the layer of n-dimensional cells is discarded when lifting to the variety). This is partly the motivation for Definition 4.3 being numbered with respect to ℓ in this way, as discussed in Remark 4.2.

Algorithm 4.5: `LayeredVarietySubCAD`$(\varphi, \mathtt{f}, \ell, \mathbf{x})$: ℓ-layered variety sub-CAD algorithm.

Input : A formula φ, a declared equational constraint $f = 0$ from φ, an integer $1 \leq \ell \leq n+1$ and variables $\mathbf{x} = x_1, \ldots, x_n$. φ is in $\mathbf{x}$ and all factors of f have main variable x_n.

Output: An ℓ-layered variety sub-CAD $\mathcal{D}$ for φ, or **FAIL**.

```
1  Extract from φ the set of polynomials A and from f the subset E ⊂ A ;
2  P ← output from applying ProjOp to (A,E) ;        // First projection stage
3  D' ← LayeredSubCAD(P, ℓ) ;          // Computation of a sub-CAD of ℝ^{n-1}
4  if D' = FAIL then
5      return FAIL ;                                  // P is not well oriented
6  D ← [];
7  for c ∈ D' do
8      S ← GenerateStack(E, c);                       // Final lifting stage
9      if S = FAIL then
10         return FAIL ;                          // Input is not well oriented
11     if |S| > 1 then
12         for i = 1 ... (|S| − 1)/2 do
13             D.append(S[2i]) ;          // Cells with even index are sections
14 return D;
```

Lemma 4.6 leads to Algorithm 4.5 for producing ℓ-layered variety sub-CADs. In Algorithm 4.5, an ℓ-layered sub-CAD of $\mathbb{R}^{n-1}$ is produced with Algorithm 4.3 (alternatively, Algorithm 4.4 could be used) which is then lifted to give a variety sub-CAD by the same method as in Algorithm 4.1.

Algorithm 4.5 has been implemented in `ProjectionCAD`, with further details in Section C.2.

Theorem 4.7.

When the sub-algorithms are chosen to implement McCallum's algorithm to produce CADs with respect to an equational constraint [McC99], then Algorithm 4.5 satisfies its specification with the output being a ℓ-layered variety sub-CAD consisting of cells on which the input formula has constant truth value.

Proof.

Much like Theorem 4.1, the structure and invariance property of the sub-CAD produced follows directly from the specifications of the sub-algorithms used (in this case, those sourced from [McC99]).

Theorem 4.2 verifies that $\mathcal{D}$ is an ℓ-layered sub-CAD of $\mathbb{R}^{n-1}$ and Lemma 4.6 concludes that the lifting in the final loop results in an ℓ-layered variety sub-CAD of $\mathbb{R}^n$. If the conditions of Lemma 4.6 do not hold, then the input is not well-oriented and thus **FAIL** is returned in line 10.

□

Example 4.4.
Consider again the unit sphere from Example 4.1. A complete CAD contains 25 cells, and we have seen that a variety sub-CAD contains 6 cells and layered sub-CADs contain 7, 17 and 23 cells for one to three layers. Constructing layered variety sub-CADs reduces these numbers further, with a 1-layered variety sub-CAD containing 2 cells (the open hemispheres) and the 2-layered variety sub-CAD containing 4 cells.

The effect is amplified if we also include the plane $x + y + z - 1$. Constructing a complete CAD creates 211 cells and an equational constraint CAD produces 137 cells. We have seen that a variety sub-CAD produces 46 cells, and layered sub-CADs produce 44, 135 and 197 cells for one to three layers. Constructing a 1-layered variety sub-CAD produces 14 two-dimensional cells, and a 2-layered variety sub-CAD produces a total of 36 cells.

4.4.2 Truth Table Invariant sub-CADs

We can combine the idea of a sub-CAD with other CAD techniques. In this section we shall discuss the interaction of layered and variety sub-CADs with projection and lifting truth table invariant CADs, which were discussed in Chapter 3 and introduced in [BDE$^+$13, BDE$^+$14].

Recall the definition of a TTICAD, given in Definition 3.2:

Definition 4.7.
Let $\Phi := \{\varphi_i\}_{i=1}^t$ be a list of quantifier-free (Tarski) formulae. We say a cylindrical algebraic decomposition $\mathcal{D}$ is **truth table invariant** (a **TTICAD**), or more specifically **Φ-truth table invariant**, if the Boolean value of each φ_i is constant (either true or false) on each cell in $\mathcal{D}$.

Sections 4.2 and 4.3 were generally concerned with sign-invariance (and order-invariance where needed for theoretical justification of the McCallum projection operator). However, the theory transfers easily to truth table invariance, and we can create **truth table invariant cylindrical algebraic sub-decompositions** (**sub-TTICADs**).

Assume we have an application concerning $\Phi = \{\varphi_i\}_{i=1}^t$, where all the φ_i have their own equational constraint. Then there exists a variety on which the solutions rest, defined by the product of the individual equational constraints (the implicit equational constraint for the problem). As with Section 4.2, for simplicity, we assume that each equational constraint has factors which all have main variable x_n. We can then define a **variety sub-TTICAD**.

Definition 4.8.
Let $\Phi := \{\varphi_i\}_{i=1}^t$ be a list of quantifier free formulae with each φ_i having equational constraint f_i whose factors all have main variable x_n. A sub-CAD of a TTICAD for Φ containing all cells resting on the variety defined by $\prod_{i=1}^t f_i = 0$ is called a **variety sub-TTICAD** (**V-sub-TTICAD**).

Algorithm 4.1 can then be used for Φ with the implicit equational constraint (the product of the individual equational constraints) being used for f. In this case `ProjOp` should be the TTICAD projection operator defined in Definition 3.4 which is applied to Φ. The `GenerateStack` procedure called on line 9 of Algorithm 4.1 should also check for the TTICAD well-orientedness condition given in Definition 3.6.

It is straightforward to give a proof analogous to that of Theorem 4.1, which shows that such an algorithm would provide a variety sub-TTICAD. Note that although the variety considered is the same as if we had constructed a sub-CAD using just the implicit equational constraint, the TTICAD theory allows for a simpler $(n-1)$-dimensional CAD, which offers further savings when lifted to the variety.

We can also create an **ℓ-layered sub-TTICAD**

Definition 4.9.
Let $\Phi := \{\varphi_i\}_{i=1}^t$ be a list of quantifier free formulae and let $1 \leq \ell \leq n+1$. A sub-CAD of a TTICAD for Φ containing all cells of dimension $n-i$ for $0 \leq i < \ell$ is called an **ℓ-layered sub-TTICAD** (**ℓ-L-sub-TTICAD**).

To construct such a sub-CAD we can use either Algorithm 4.3 or Algorithm 4.4 by using the TTICAD projection operator and a `GenerateStack` algorithm which checks for the TTICAD well-orientedness condition of Definition 3.6 (as with constructing a variety sub-TTICAD). Again, the validity follows an analogous proof to the sub-CAD algorithm, in this case Theorems 4.2 and 4.3.

Finally, we can combine TTICAD theory with the idea in Section 4.4.1 to produce a layered variety sub-TTICAD, as specified in the following definition.

Definition 4.10.
Let $\Phi := \{\varphi_i\}_{i=1}^t$ be a list of quantifier free formulae with each φ_i having equational constraint f_i whose factors all have main variable x_n. Let $1 \leq \ell \leq n$. A sub-CAD of a TTICAD for Φ containing all cells of dimension $n-1-i$ for $0 \leq i < \ell$ resting on the variety defined by $\prod_{i=1}^t f_i = 0$ is called a **ℓ-layered variety sub-TTICAD** (**ℓ-LV-sub-TTICAD**).

Remark 4.6.
As with ℓ-layered variety sub-CADs (Definition 4.6), an ℓ-layered variety sub-TTICAD consists of the top ℓ layers of cells on the variety (in this case defined by $\prod_{i=1}^t f_i = 0$). This can be thought of as the intersection of an $(\ell+1)$-layered sub-CAD of $\mathbb{R}^n$ with the variety (with the n-dimensional cells being discarded when lifting to the variety).

Constructing a layered variety sub-TTICAD can be done using Algorithm 4.5 with the sub-algorithms (for projection and stack generation) being those needed for TTICAD theory. The correctness follows, again, analogously to that of layered variety sub-CADs which was given in Theorem 4.7 (relying on the sub-TTICAD versions of Theorems 4.1, 4.2 and 4.3). The exceptional case when part of the variety is nullified on a cell will be identified by the TTICAD algorithms and will therefore produce **FAIL**.

All three algorithms described in this section (to produce variety sub-TTICADs, layered sub-TTICADs, and layered variety sub-TTICADs) have been implemented in the `ProjectionCAD` package, which is discussed further in Section C.2.

4.5 Complexity of Variety sub-CADs

In this section we extend the work of Collins ([Col75]) and McCallum ([McC93]) regarding complexity of CAD algorithms. We give a complexity analysis of the algorithms to compute sign-invariant variety sub-CADs (Algorithm 4.1) and 1-layered variety sub-CADs (Algorithm 4.5) in the specific case where the equational constraint has all factors with main variable x_n.

We need to consider three parts of the complexity for the sub-CADs:

Projection The complexity of the equational constraint projection set needs to be analysed. In particular the number of polynomials, the maximum degree and size of their coefficients.

Calculation of $(n-1)$ dimension CAD/sub-CAD These values then can be used to estimate the complexity of the $(n-1)$–dimensional CAD or sub-CAD.

Lifting Finally the complexity of the lifting stage can be combined with the previous step to describe the complexity of the variety sub-CADs.

We first standardise some notation for a CAD with respect to a set of polynomials A (with equational constraint set $E \subseteq A$): let n be the number of variables, m the number of polynomials in A, d the maximum degree in any variable of the polynomials in A, and l the maximum norm length of the polynomials in A (where the **norm length**, $|f|_1$, is the sum of the absolute values of the integer coefficients of a polynomial).

Let $A_1 := A$ and let $A_{i+1} := \text{Proj}(A_i)$. In general the projection operator used will be clear: most of the following is with respect to Collins' projection operator $_{\mathbf{C}}\mathbf{P}$ (Definition 2.22) and, therefore, is a 'worst case scenario' compared to the improved operators of McCallum $_{\mathbf{M}}\mathbf{P}$ (Definition 2.24) and Brown $_{\mathbf{BM}}\mathbf{P}$ (Definition 2.27), which are both subsets of the Collins operator. Let m_k be the number of polynomials in A_k, d_k the maximum degree of A_k, and l_k the maximum norm length.

4.5.1 Collins' algorithm

In [Col75], Collins works through his original CAD algorithm in great detail to analyse the complexity, and this methodology is followed in [McC93] when discussing the 1-layered CAD algorithm. We recall some key results, noting they could all be uniformly improved with ideas from papers such as [Bur13, Dav85] but the aim of this section is not to achieve tighter complexity bounds for existing algorithms, but rather to give complexity bounds for sub-CADs in the context of existing results.

In the projection stage the properties of the projection sets can be bound as follows:

$$m_k \leq (2d)^{3^k} m^{2^{k-1}}; \quad d_k \leq \frac{1}{2}(2d)^{2^{k-1}}; \quad l_k \leq (2d)^{2^k} l.$$

By combining these bounds Collins shows the projection phase is dominated by

$$(2d)^{3^{n+1}} m^{2^n} l^2.$$

The base case and lifting algorithm requires the isolation of real roots of univariate polynomials. Collins bounds this procedure as follows. Let A be a set of univariate polynomials with degree bounded by d and norm length bounded by l. Then for a given $f \in A$ with $\hat{d} := \deg(f)$ and $\hat{l} := |f|_1$ a lower bound on the distance between two roots is given by

$$\frac{1}{2}\left(\sqrt{e}\hat{d}^{\frac{3}{2}}\hat{l}\right)^{-\hat{d}}. \tag{4.1}$$

Collins uses his analysis of Heindel's algorithm for real root isolation to show that isolating the roots is dominated by

$$\hat{d}^8 + \hat{d}^7\hat{l}^3. \tag{4.2}$$

Therefore the number of operations needed to isolate all roots in A, with $m := |A|$, is dominated by:

$$md^8 + md^7l^3. \tag{4.3}$$

For a given h, refining a root interval to 2^{-h} is dominated by $d^2h^3 + d^2l^2h$. Collins multiplies all polynomials in A and uses (4.1) to show that all roots are separated by:

$$\delta := \frac{1}{2}\left(\sqrt{e}(md)^{\frac{3}{2}}l^m\right)^{-md}.$$

If we take h to be $\log(\delta)$ we can refine all intervals of the polynomials in

$$md(d^2(m^2dl + md\log(md))^3 + md^3l^3) = O(m^7d^7l^3 + m^2d^4l^3).$$

Combining this with (4.3) tells us that the necessary refinement of intervals for all the polynomials is dominated by

$$md^8 + m^7d^7l^3. \tag{4.4}$$

Remark 4.7.
Whilst discussing this work for publication in [BDE+14] the authors noted that the analysis to obtain (4.4) can be improved using recent advances in root isolation.

In [Dav85] it was noted that it is unnecessary to consider the product of all polynomials when computing δ, two polynomials will suffice. Therefore δ becomes:

$$\delta := \frac{1}{2}\left(\sqrt{e}(2d)^{\frac{3}{2}}l^2\right)^{-2d}.$$

As we take h to be $\log(\delta)$ this now becomes $2d(2l + \log d)$ (which is $\tilde{O}(dl)$). Substituting into the interval separation bound gives $md^6l^3 + md^4l^3$. We see this is dominated by (4.3) and so (4.3) dominates the overall complexity:

$$md^8 + md^7l^3. \tag{4.5}$$

In [Bur13] the author states that (4.2) can be improved to $\tilde{O}(d^4l^2)$. We therefore have (4.3) bounded by $\tilde{O}(md^4l^2)$ and we can combine this with the reasoning in [Dav85]

to obtain an overall bound of:

$$md^4l^2 + md(d^5l^3 + d^3l^3) = \tilde{O}(md^6l^3). \tag{4.6}$$

We can also apply [Bur13] to the product of all polynomials in A to immediately isolate all roots. This gives a better estimate for (4.4):

$$(md)^4(mdl)^2 = m^6d^6l^2. \tag{4.7}$$

Using any of (4.5), (4.6), and (4.7) in Collins' analysis will filter through to the overall complexity, reducing the exponents produced. This would not provide any great new insight into the algorithms and so we do not go into details here. The subsequent work continues to follow Collins' original reasoning.

Combining (4.4) with the size of the full projection set concludes the base phase is dominated by

$$(2d)^{3^{n+3}}m^{2^{n+2}}l^3.$$

We now need to consider the polynomials involved in the lifting stage. This involves looking at the univariate polynomials created after substituting sample points, along with the polynomials required to define the algebraic extensions of $\mathbb{Q}$ that those sample points are contained in.

We follow the work in [Col75, McC93] by using primitive elements to calculate the costs of operations, even though these are unlikely to be used by implementations. For each sample point $\beta = (\beta_1, \ldots, \beta_k) \in \mathbb{R}^k$ there is a real algebraic number $\alpha \in \mathbb{R}$ such that $\mathbb{Q}(\beta_1, \ldots, \beta_k) = \mathbb{Q}(\alpha)$. Let f_α be the polynomial in $\mathbb{Q}[x]$ that, along with an isolating interval I_α, defines α (so $f(\alpha) = 0$). Let d_k^* be the maximum degree of these f_α, and l_k^* the maximum norm length. Each coordinate β_i is represented in $\mathbb{Q}(\alpha)$ by another polynomial. Let l_k' be the maximum norm length of these polynomials. Then

$$d_k^* \leq (2d)^{2^{2n-1}}, \quad \text{and} \quad l_k^*, l_k' \leq (2d^2)^{2^{2n+3}}m^{2^{n+1}}l.$$

Let u_k be the number of univariate polynomials (after substitution) and c_k the number of cells at level k. Then

$$u_k, c_k \leq 2^{2^n}\prod_{i=1}^{n} m_i d_i, \quad \text{and} \quad u_k, c_k \leq (2d)^{3^{n+1}}m^{2^n}. \tag{4.8}$$

Collins combines all these results to give a complexity bound for the full algorithm of

$$(2d)^{4^{n+4}} m^{2^{n+6}} l^3. \tag{4.9}$$

4.5.2 McCallum's CADMD algorithm

In [McC93], McCallum introduces his CADMD algorithm which constructs a 1-layered sub-CAD (which he refers to as a CAD of maximal dimension) in the same manner as Algorithm 4.3 with $\ell = 1$. Using the same methodology as [Col75], he gives a complexity bound for the CADMD algorithm. As constructing a 1-layered CAD avoids using algebraic numbers (all cells are direct products of intervals so sample points can be produced directly in $\mathbb{Q}$) the exponents in the complexity are lower than in (4.9). The complexity is dominated by:

$$(2d)^{3^{n+4}} m^{2^{n+4}} l^3. \tag{4.10}$$

4.5.3 Analysis of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ and $(n-1)$-dimensional CADs

We need to consider properties of the projection set to consider the complexity of the sub-CADs produced: the size, maximum degree and maximum norm length. Let $E \subseteq A$ be the subset of A containing the factors of the designated equational constraint (for which the variety sub-CAD will be construct with respect to). Define the following parameters:

$$m_A := |A|, \quad m_E := |E|, \quad m_{A\setminus E} := |A \setminus E|.$$

Let d_A, d_E, $d_{A\setminus E}$ be the maximum degrees of the relevant sets, and let l_A, l_E, $l_{A\setminus E}$ be the maximum norm length of each set.

We are constructing a sub-CAD with respect to an equational constraint so we use the projection operator ${}_{\mathbf{M}}\mathbf{P}_E(A)$ defined by McCallum (Definition 2.32 and originally given in [McC99]). Recall that the definition of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ is:

$${}_{\mathbf{M}}\mathbf{P}_E(A) := {}_{\mathbf{M}}\mathbf{P}(E) \cup \{\mathrm{res}_{x_n}(f,g) \mid f \in E, g \in A \setminus E\}$$

where ${}_{\mathbf{M}}\mathbf{P}(E)$ is the McCallum projection operator defined in [McC85, McC98] (Definition 2.24) which gives the coefficients, discriminants and cross resultants of E. We will denote the resultant set, ${}_{\mathbf{M}}\mathbf{P}_E(A) \setminus {}_{\mathbf{M}}\mathbf{P}(E)$, by $\mathrm{ResSet_E(A)}$.

We can bound the size of ${}_{\mathbf{M}}\mathbf{P}(E)$ by the sum of the sizes of its components: the number of coefficients (bounded by $m_E d_E$), the number of discriminants (bounded by m_E), and the number of resultants (bounded by $\binom{m_E}{2} = \frac{m_E(m_E-1)}{2}$). Note that in

practice a fraction of these elements will be trivial with respect to constructing a CAD (either 0 or a constant) hence we can only use these numbers as bounds. Combining these bounds gives:

$$\begin{aligned}|{}_{\mathbf{M}}\mathbf{P}_E(A)| &\leq m_E d_E + m_E + \frac{m_E(m_E-1)}{2} + m_E m_{A\setminus E} \\ &= \frac{m_E}{2}\left(2d_E + 2m_{A\setminus E} + m_E - 1\right) \\ &= \frac{m_E}{2}\left(2d_E + m_{A\setminus E} + m_A - 1\right). \end{aligned} \tag{4.11}$$

The maximum degree of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ is the greater of the maximum degrees of ${}_{\mathbf{M}}\mathbf{P}(E)$ and the resultant set. We also have the following standard bound [VZGG13, Thm 6.22] on the degree of a resultant with respect to x (where $f, g \in \mathbb{K}[x, y]$):

$$\deg(\mathrm{res}_x(f,g)) \leq (\deg_x f + \deg_x g) \cdot (\max(\deg_y f, \deg_y g)).$$

Using our overall degree bounds gives

$$\begin{aligned}\max\deg(\mathrm{ResSet}_E(A)) &\leq (d_E + d_{A\setminus E}) \cdot \max(d_E, d_{A\setminus E}) \\ &= \max(d_E^2 + d_E d_{A\setminus E}, d_{A\setminus E}^2 + d_E d_{A\setminus E}) \\ &\leq \max(2d_E^2, 2d_{A\setminus E}^2). \end{aligned} \tag{4.12}$$

We also have

$$\max\deg({}_{\mathbf{M}}\mathbf{P}(E)) \leq \max(d_E, 2d_E^2, 2d_E^2) = 2d_E^2. \tag{4.13}$$

Combining (4.12) and (4.13) gives a degree bound for ${}_{\mathbf{M}}\mathbf{P}_E(A)$:

$$\max\deg({}_{\mathbf{M}}\mathbf{P}_E(A)) \leq \max(2d_E^2, 2d_{A\setminus E}^2) \leq d_A^2. \tag{4.14}$$

Finally, if we denote the maximum norm length of ${}_{\mathbf{M}}\mathbf{P}_E(A)$ by $\bar{l}$, then we know $\bar{l} \leq l_2$ (since ${}_{\mathbf{M}}\mathbf{P}_E(A) \subseteq {}_{\mathbf{M}}\mathbf{P}(A) \subseteq {}_{\mathbf{C}}\mathbf{P}(A)$) and so

$$\bar{l} \leq l_2 \leq (2d_A)^{2^2} l_A = 16 d_A^4 l_A. \tag{4.15}$$

Substituting these bounds ((4.11), (4.14) and (4.15)) into (4.9) gives an estimate on the complexity of a complete $(n-1)$-dimensional ${}_{\mathbf{M}}\mathbf{P}_E(A)$-invariant Collins CAD. We

see the complexity is dominated by

$$\leq \left(2 \cdot 2d_A^2\right)^{2^{2(n-1)+8}} \left(\frac{m_E(2d_E + m_A + m_{A\setminus E} - 1)}{2}\right)^{2^{n-1+6}} \left(16d_A^4 l_A\right)^3$$
$$\leq 16^3 \left(4d_A^2\right)^{2^{2n+6}} \left(\frac{m_E(2d_E + 2m_A - 1)}{2}\right)^{2^{n+5}} l_A^3 d_A^{12}. \tag{4.16}$$

Similarly, the complexity of a 1-layered $(n-1)$-dimensional ${}_{\mathbf{M}}\mathbf{P}_E(A)$-invariant sub-CAD can be considered by substituting into (4.10). We see that the complexity of such a sub-CAD is dominated by

$$\leq \left(2 \cdot 2d_A^2\right)^{3^{n-1+4}} \left(\frac{m_E(2d_E + m_A + m_{A\setminus E} - 1)}{2}\right)^{2^{n-1+4}} \left(16d_A^4 l_A\right)^3$$
$$\leq 16^3 \left(4d_A^2\right)^{3^{n+3}} \left(\frac{m_E(2d_E + 2m_A - 1)}{2}\right)^{2^{n+3}} l_A^3 d_A^{12}. \tag{4.17}$$

4.5.4 Overall complexities for variety sub-CADs

We have so far computed bounds for the complexities of the $(n-1)$-dimensional CADs and sub-CADs produced in Algorithm 4.1 (line 4) and Algorithm 4.5 (line 3).

We now need to consider the final step of lifting over these cells with respect to the factors of the equational constraint. We can use (4.8) to bound the number of univariate polynomials so know from (4.4) that the isolations will be dominated by:

$$(2d_E)^{3^{n+1}} m_E^{2^n} d_E^8 + \left((2d_E)^{3^{n+1}} m_E^{2^n}\right)^7 d_E^7 l_E^3. \tag{4.18}$$

Remark 4.8.
We could also use the improvements of (4.5), (4.6), and (4.7) in this final lifting stage but for the sake of consistency use (4.4).

We now have the components needed to describe the overall complexities of constructing a variety sub-CAD and 1-layered variety sub-CAD. We can combine (4.18) with (4.16) and (4.17) to obtain a single bound for each. Note that (4.18) will be a large overestimation for the 1-layered case.

Theorem 4.8.
The complexity for computing a variety sub-CAD with Algorithm 4.1 using ${}_{\mathbf{M}}\mathbf{P}_E(A)$ *and*

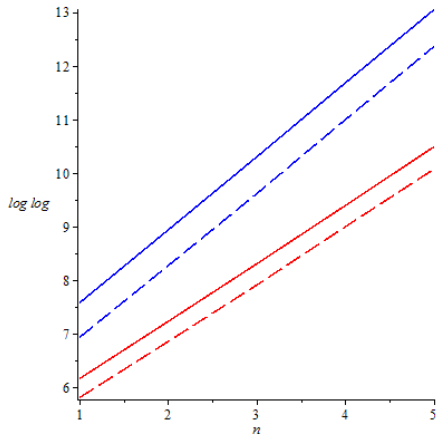


Figure 4.1: A plot of n against the double logarithm of the complexities of algorithms. The complexities were evaluated with parameter choices $d_A = 3$, $d_E = 2$, $m_A = 3$, $m_E = 1$, $m_{A\setminus E} = 2$, $l_A = 2$, $l_E = 2$. From top to bottom the complexities are given for a complete CAD, a variety sub-CAD, a 1-layered sub-CAD and a 1-layered variety sub-CAD.

Collins' algorithm is dominated by:

$$2^{12}\left(2^2 d_A^2\right)^{\mathbf{4^{n+3}}}\left(\frac{m_E(2d_E+2m_A-1)}{2}\right)^{\mathbf{2^{n+5}}} l_A^3 d_A^{12} + (2d_E)^{3^{n+1}} m_E^{2^n} d_E^8 + \left((2d_E)^{3^{n+1}} m_E^{2^n}\right)^7 d_E^7 l_E^3. \quad (4.19)$$

The complexity for computing a 1-layered variety sub-CAD using Algorithm 4.5 using ${}_{\mathbf{M}}\mathbf{P}_E(A)$ *and Collins' algorithm is dominated by:*

$$2^{12}\left(2^2 d_A^2\right)^{\mathbf{3^{n+3}}}\left(\frac{m_E(2d_E+2m_A-1)}{2}\right)^{\mathbf{2^{n+3}}} l_A^3 d_A^{12} + (2d_E)^{3^{n+1}} m_E^{2^n} d_E^8 + \left((2d_E)^{3^{n+1}} m_E^{2^n}\right)^7 d_E^7 l_E^3. \quad (4.20)$$

4.5.5 Comparison of complexities

In Theorem 4.8 key exponents have been placed in bold to highlight the difference between (4.19) and (4.20). It can be difficult to visualise the comparison therefore Figure 4.1 plots the double logarithm of the complexities of various CAD and sub-CAD algorithms against n with the following parameter values: $d_A = 3$, $d_E = 2$, $m_A = 3$, $m_E = 1$, $m_{A\setminus E} = 2$, $l_A = 2$, $l_E = 2$.

Figure 4.1 shows, from top to bottom:

- Collins' complexity for a complete CAD (4.9);
- McCallum's complexity for a 1-layered CAD (4.10);
- Theorem 4.8 complexity for a variety sub-CAD (4.19);
- Theorem 4.8 complexity for a 1-layered variety sub-CAD (4.20).

Figure 4.1 shows clearly the drop in the constant in the exponents of (4.19) and (4.20), whilst the scaling factor of the exponent remains the same between variety and non-variety versions of each algorithm.

4.6 Examples and Experimentation

We now discuss some experimental results that demonstrate the benefit of the new sub-CAD algorithms. Algorithms 4.1, 4.2, 4.3, 4.5, and the respective algorithms for sub-TTICADs have all been implemented in the `ProjectionCAD` package for Maple (further details are given in Section C.2 and [Eng13a, Eng13b, WE13]).

We compare these with competing CAD implementations. We use the two CAD procedures implemented in the `RegularChains` library for Maple: computing CADs directly ([CMXY09] and described in Section 2.5.2) and incrementally ([CM12] and described in Section 2.5.3) using regular chains technology. We use Qepcad both with its default settings (which implements McCallum's algorithm from [McC85, McC98] and described in Algorithm 2.4) and also using equational constraint technology whenever appropriate (using the theory from [McC99] described in Section 2.32). Finally, we use the algorithms available in Mathematica, which produce cylindrical algebraic formulae rather than CADs.

It is worth noting that Qepcad offers an option `measure-zero-error` which will produce a CAD for which only the full-dimensional cells of the free variable space are guaranteed to satisfy the specified invariance condition (normally truth invariance of the input formula). The output of Qepcad is always a CAD, but this option clearly has parallels with sub-CAD theory, namely 1-layered sub-CADs. More specifically, if we only retain those cells for which the invariance condition is guaranteed to be correct then we would have a 1-layered sub-CAD, and therefore all solutions up to an error set of measure zero, in the free-variable space.

For the experiments below this command cannot be used: we consider unquantified formulae (so the free variable space is n-dimensional) and each has an equational

constraint. Therefore the specified formulae can only be satisfied on cells with dimension strictly less than n. If we use the `measure-zero-error` option with QEPCAD then the only cells guaranteed to be correct have dimension n and are therefore not of interest. When we construct a 1-layered variety sub-CAD (using the implementation of `ProjectionCAD`) we do obtain solutions: here the layer is with respect to the variety, and not free variable space. Therefore a 1-layered variety sub-CAD provides solutions correct up to an error set of measure zero in the solution space.

The following experiments were run on the same configuration as the rest of this thesis: a Linux desktop (3.1GHz Intel processor, 8.0Gb total memory). The MATHEMATICA used was Version 9 and QEPCAD-B 1.69 was used with the options `+N500000000` and `+L200000` (initialisation times are included in all results and are generally around 2 seconds). The development version of MAPLE is used in command line interface, using the development version of the `RegularChains` Library.

4.6.1 Example: Making use of a 1-layered variety sub-CAD

We work through an example to show the benefit of a 1-layered variety sub-CAD.

Example 4.5.
Assume variable ordering $x \succ y \succ z$ and consider the following formula which was created using 3 random polynomials of degree 2 (generated using MAPLE's `randpoly` function) which are plotted in Figure 4.2:

$$\begin{aligned}\Phi := -50xy + 56yz + 41z^2 + 67x - 55y - 21 = 0 \\ \wedge \quad 36xy + 76xz - 58yz + 69z^2 + 75y + 27 > 0 \\ \wedge \quad -55x^2 + 10xy - 88x + 80y + z - 39 > 0.\end{aligned}$$

For a given problem we may wish to describe the regions of $\mathbb{R}^3$ in which Φ is satisfied. Figure 4.2 shows there are multiple intersections between the two non-equational constraints away from the variety defined by the equational constraint (shown in red). This suggests that a variety sub-CAD would be beneficial over a complete CAD. We can obtain further savings if only generic solutions are required by constructing a 1-layered variety sub-CAD.

We attempt to solve the given problem with a variety of theories to show the relative benefits of each. We compute:

- a complete sign-invariant CAD for the three polynomials in Φ using McCallum's projection operator (`CADFull`: Algorithm 2.4);

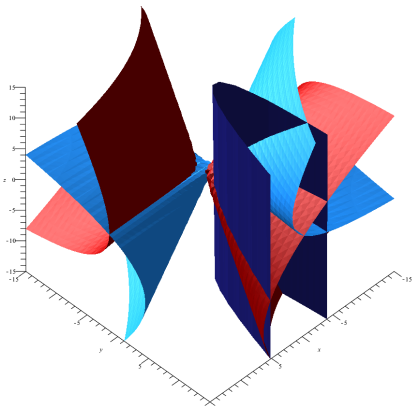


Figure 4.2: Intersection of the three surfaces from Section 4.6.1. The red surface is the equational constraint.

Technique	Cells	Time
`CADFull`	17047	178.277
`ECCAD`	1315	11.520
V-sub-CAD	422	10.723
2-LV-sub-CAD	348	7.149
1-LV-sub-CAD	138	0.475
RC-Rec-CAD	9841	112.460
RC-Inc-CAD	559	1.999
QEPCAD	17047	385.679
EC-QEPCAD	5271	26.614
MATHEMATICA	—	0.533

Table 4.1: Constructing sub-CADs and CADs for Φ with various algorithms.

- an equational constraint CAD (`ECCAD`: McCallum's theory of equational constraints [McC99]);
- a variety sub-CAD (V-sub-CAD: Algorithm 4.1 using sub-procedures following McCallum's theory of equational constraints in [McC99]);
- layered variety sub-CADs (LV-sub-CAD: Algorithm 4.5 using sub-procedures following McCallum's theory of equational constraints in [McC99]).

The cell counts and timings to compute such CADs and sub-CADs with `ProjectionCAD` are given in the first half of Table 4.1.

It is clear that utilising the equational constraint dramatically reduces computation

time and the number of cells produced. Restricting to a variety sub-CAD increases this cell saving further, which will lead to even more significant time savings on any subsequent work using the cells of the sub-CAD. The variety sub-CAD describes all solutions to Φ, but we can also use the 1-layered variety sub-CAD to describe the generic solutions in a much quicker time (any valid cells not in this sub-CAD will have measure zero in the solution space). Therefore in this case, an output of 17,047 cells can be replaced with only 138 cells. If we need to describe the other solutions then a 2-layered variety sub-CAD or complete variety sub-CAD will only produce 348 and 422 cells respectively.

We compare these computation times and cell counts with the current state-of-the-art implementations of CAD algorithms, which are given in the second half of Table 4.1. As with the algorithms from `ProjectionCAD`, we see that taking advantage of equational constraints (in the incremental CAD of `RegularChains`, RC-Inc-CAD, and QEPCAD, EC-QEPCAD) offers a large cell saving and significant reduction in speed. Comparatively, QEPCAD performs worse here than the other implementations both in terms of time and, when using equational constraints, cell count. This is perhaps due to the fact QEPCAD does not implement the improved lifting offered by equational constraint theory (described in Remark 3.1 and implemented in `ProjectionCAD`).

In both of the CADs produced by QEPCAD, Φ is valid only a small fraction of the cells produced. For the sign-invariant CAD only 290 cells from the 17,047 cells produced are valid (1.7%) and for the equational constraint CAD 106 cells are valid from the 5271 cells produced (2.0%). Such a large volume of false cells that are unnecessarily constructed (and on which the polynomials in Φ are evaluated) explains the larger computation times.

To offer a comparison, we can very quickly evaluate Φ on the cells of the 1-layered variety sub-CAD. Of the 138 cells produced, we see that 36 of them describe solutions to Φ (26.1%). Without a full implementation of evaluating polynomials at algebraic sample points described by nested `RootOf` constructs we cannot accurately determine the fraction of valid cells for the remaining sub-CADs.

As noted in all our experimentation, MATHEMATICA produces cylindrical formulae rather than CAD cells and so a direct comparison is difficult. Obviously the speed at which MATHEMATICA computes a cylindrical formula for Φ is impressive, but we cannot infer any general behaviour from it.

Remark 4.9.
QEPCAD allows for the `measure-zero-error` option to be used for Φ along with declaring

the equational constraint. Enabling both options allows QEPCAD to produce a CAD in under 5 seconds with 822 cells. However, as the solution space of Φ is at most $(n-1)$-dimensional, none of the full dimensional cells satisfy Φ and so QEPCAD returns an equivalent quantifier free formula of `False`.

In general we could consider a problem of the form $f = 0 \wedge \Psi(g_i)$ where $f = 0$ defines a variety of real co-dimension 1 and Ψ is a quantifier-free formula involving only $f = 0$ and strict inequalities in the g_i. Then a 1-layered variety sub-CAD will, in most cases, be sufficient to describe the generic solutions for the given problem. There will need to be checks for nullification, and there may be no solutions of full dimension on the variety, in which case the recursive approach for layered sub-CADs can be used to incrementally build successive layers until a solution is found (or the entire variety sub-CAD is constructed and no solutions are possible).

4.6.2 Example: Making use of 1-layered variety sub-TTICAD

We now demonstrate the strength of sub-TTICADs with another example.

Example 4.6.
Consider the following quantifier free formulae:

$$\begin{aligned}\varphi_1 &:= x^2 + y^2 + z^2 = 1 \wedge xy + yz + zx < 1 \wedge x^3 - y^3 - z^3 < 0;\\ \varphi_2 &:= (x-1)^2 + (y-1)^2 + (z-1)^2 = 1 \wedge (x-1)(y-1) + (y-1)(z-1)\\ &\qquad + (z-1)(x-1) < 1 \wedge (x-1)^3 - (y-1)^3 - (z-1)^3 < 0.\end{aligned}$$

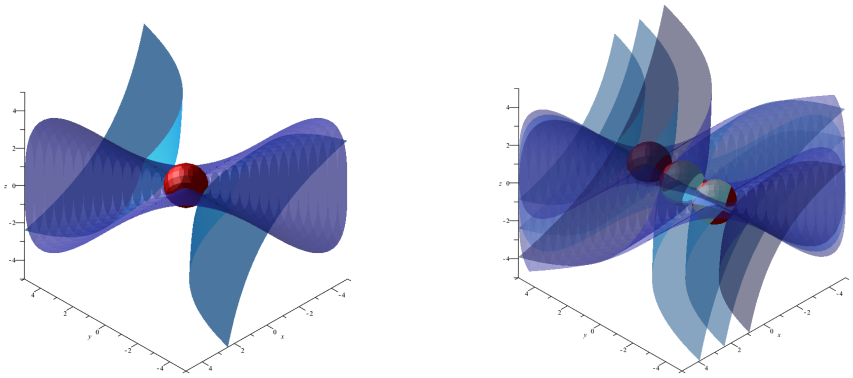
The surfaces of φ_1 are shown in Figure 4.3a, with the equational constraint indicated in red (the surfaces of φ_2 are the same but translated by the vector $(1,1,1)$).

We assume the variable ordering $x \succ y \succ z$ and construct the following formula, Φ, defining regions of $\mathbb{R}^3$:

$$\Phi := \varphi_1 \vee \varphi_2.$$

This problem is deceptively difficult to tackle directly with a sign-invariant CAD for Φ: running the default CAD algorithm in MAPLE 16 (recursive regular chains CAD as described in [CMXY09]) overnight fails to produce any output, and QEPCAD hits a memory constraint ("prime list exhausted") after two hours of computation.

We can make some use of the equational constraints of φ_1 and φ_2. In QEPCAD we can declare the implicit equational constraint (the product of the two spheres) which takes $35,304$ seconds (about 10 hours) to produce a CAD with $6,165$ cells. MATHEMATICA can



(a) Intersection of the surfaces from φ_1. (b) Intersection of the surfaces from Φ^*.

Figure 4.3: Intersection of the surfaces from φ_1 and Φ^* in Example 4.6. The spheres defined by the equational constraints are shown in red.

produce a relevant cylindrical formula in 1.805 seconds but it is not possible to inspect the number of cells constructed.

Clearly Φ is well-suited for TTICAD and so we can use the implementation in `ProjectionCAD`. Doing so produces $4,861$ cells in 170.515 seconds: a lower cell count than QEPCAD is obtained due to the improved TTICAD projection operator and improved lifting (discussed in Section 3.2.1 and Remark 3.1).

We now consider how to obtain a more efficient output using the sub-TTICAD theory discussed in Section 4.4.2. Both φ_1 and φ_2 contain an equational constraint and so any region where Φ is valid must lie on the variety defined by the product of the equational constraints. If we only require generic solutions then we can construct a 1-layered variety sub-TTICAD for this variety.

To start, we project φ_1 and φ_2 with respect to the TTICAD projection operator (Definition 3.4) and use these projection polynomials to construct a 1-layered sub-CAD of $\mathbb{R}^2$: 249 cells are produced in 0.947 seconds. We then lift using both equational constraints retaining only those cells on the variety, taking a further 1.191 seconds and producing 528 2-dimensional cells on the 2-dimensional variety in $\mathbb{R}^3$. The 1-layered variety sub-TTICAD therefore reduced the number of cells by 88% and construction time by 99% compared to a full TTICAD, producing those generic solutions of two dimensions (as φ_1 and φ_2 contain strict inequalities alongside the equational constraints it is likely that there will be relatively few solution regions of smaller dimension). If we require solutions of lower dimension then we can construct a 2-layered variety sub-TTICAD with $1,514$ cells in 47.629 seconds.

If we require all solutions then we can construct a variety sub-TTICAD which will produce $1,976$ cells in 178.196 seconds. A variety sub-TTICAD therefore takes approximately the same time to compute as a full TTICAD but gives a substantial cell saving of 59% fewer cells (indicating that over half the cells in the complete TTICAD do not lie on either of the varieties defined by the equational constraints).

We can include a third formula (another shift of φ_1 but with respect to $(-1,-1,-1)$):

$$\begin{aligned}\varphi_3 := (x+1)^2 + (y+1)^2 + (z+1)^2 = 1 \wedge (x+1)(y+1) + (y+1)(z+1) \\ + (z+1)(x+1) < 1 \wedge (x+1)^3 - (y+1)^3 - (z+1)^3 < 0,\end{aligned}$$

and combine it with Φ to produce a new formula:

$$\Phi^* := \varphi_1 \vee \varphi_2 \vee \varphi_3.$$

The nine surfaces of Φ^* are shown in Figure 4.3b, with the spheres, which are the equational constraints, shown in red.

It is impractical to attempt to build a CAD for Φ^* without using equational constraints (as the CAD will be strictly finer than a sign-invariant CAD for Φ, which was shown to be infeasible). Although the problem is significantly more complicated, constructing a 1-layered variety sub-TTICAD takes only 5.003 seconds and produces $1,104$ cells. A 2-layered variety sub-TTICAD produces $3,166$ cells in 145.898 seconds; a variety sub-TTICAD produces $4,130$ cells in 429.083 seconds. By comparison a complete TTICAD takes about the same time as a variety sub-TTICAD (432.210 seconds) but produces over double the cells ($10,063$ cells).

4.7 Extensions to the Theory

Variety and layered sub-CADs are not the only possible ways to construct a sub-CAD, and in Section 4.1.1 a variety of related work in the literature was discussed. We now discuss a variety of ways the theory of sub-CADs could be extended.

4.7.1 Restricted Lifting Over Simple Inequalities

Often a CAD problem sourced from a real world example will contain many simple inequalities. This is primarily as we rarely want a variable to range over the entirety of the reals, but rather an interval.

Algorithm 4.6: `BasicSimpleInequalitysubCAD(F, vars)`: Basic simple inequalities sub-CAD algorithm.

Input : A formula Φ, a set of variables $vars = x_1, \ldots, x_n$.
Output: A sub-CAD with respect to the inequalities in the variable of $\mathbb{R}^1$.

```
1  E ← EqConst(Φ); I ← IneqConst(Φ);              // Separate inequalities
2  P ← ProjOp(Φ, vars);
3  D_1 ← SplitR(P[n]);
4  I ← {};
5  for f ∈ E ∪ I do
6      I.append(InferIneq(f, x_1));               // Obtain inequalities in x_1
7  I' ← combine(I);                  // Combine and simplify inequalities
8  D'_1 ← refine(D_1, I);            // Restrict according to inequalities
9  D ← lift(P, vars, D_1);                        // Continue lifting phase
10 return D;
```

There are multiple extensions to CAD theory (such as equational constraints or TTICAD) that concentrate on utilising the power of equational constraints, and the idea behind variety sub-CADs is also centred around this, but relatively little research into using these simple inequalities directly. They will certainly be used within partial CAD [CH91] and the authors of SyNRAC have commented on their use within formula simplification [YA04]. We now describe an idea to extend how inequalities are used in partial CAD to produce sub-CADs.

In [McC97] (which will be discussed further in Section 6.3) the author considers a problem that is infeasible when tackled directly with CAD. To make the problem feasible, the author derives a simple inequality for the variable, r, which decomposes $\mathbb{R}^1$. As the formula involves the equational constraint $r^2 + s^2 = -1$ the author notes that $-1 \leq r \leq 1$ must hold. Manually selecting those cells that satisfy this inequality, the author lifts only over that region, producing a sub-CAD of $\mathbb{R}^4$ (which is a complete CAD of $[0, 1] \times \mathbb{R}^3$).

This can easily be incorporated into a general algorithm, as shown in Algorithm 4.6.

Example 4.7.
We consider a simple example to show the power of utilising simple inequalities in the lifting stage. Consider the following formula:

$$\left[[x^2 + y^2 + z^2 * 1] \wedge [x > 0] \wedge [y > 0] \wedge [z > 0]\right], \quad * \in \{=, \neq, <, >, \leq, \geq\}.$$

This will define a property of the positive octant of the unit sphere. Were we to construct

a full CAD using McCallum's projection operator for $\{x^2+y^2+z^2-1, x, y, z\}$, we would construct 135 cells.

Using the basic inequality sub-CAD algorithm described in Algorithm 4.6 constructs 51 cells. At the base-CAD level the only cells retained are $0 < x < 1$, $x = 1$, $x > 1$. The following liftings have the savings:

- **1-D sub-CAD:** 7 cells are reduced to 3 cells;
- **2-D sub-CAD:** 33 cells are reduced to 13 cells;
- **3-D sub-CAD:** 135 cells are reduced to 51 cells.

Constructing a partial CAD would have the 51 cells of the basic inequality sub-CAD, along with four trivial cells: $[x = 0] \times \mathbb{R}^2$, $[-1 < x < 0] \times \mathbb{R}^2$, $[x = -1] \times \mathbb{R}^2$, and $[x < -1] \times \mathbb{R}^2$. These may get simplified with post-processing [Bro98] although there will always be at least 1 extra cell (as a partial CAD is still a complete decomposition of $\mathbb{R}^n$).

Ideally, we would want to incorporate simple inequalities into every level of cells: when lifting from $\mathbb{R}^{k-1}$ to $\mathbb{R}^k$, only retain cells which satisfy the simple inequalities that can be inferred from the input formula. Often every variable will be considered on a restricted domain, and so the savings could be substantial.

If the only inequalities considered are truly trivial (of the form $x_k < \alpha$ or $x_k \leq \alpha$ for $\alpha \in \mathbb{R}$, or preferably $\alpha \in \mathbb{Q}$) then this should be possible at all levels. The endpoints will be explicitly identified (for an inequality $x_k < \alpha$, the polynomial $x_k - \alpha$ will appear in the projection set) and therefore when lifting over a cell from $\mathbb{R}^{k-1}$ there will be a cell with $x_k = \alpha$ (both in the cell representation and sample point). The stack can then be restricted appropriately in relation to this cell. This process should be relatively inexpensive and could offer large savings. Care needs to be taken when there are nested algebraic numbers, as demonstrated in the issues of implementing quantifier elimination via CAD.

We demonstrate how such an algorithm could offer large savings over both a general CAD algorithm, and a partial CAD implementation.

Example 4.8.
Consider again the formula:

$$\left[[x^2 + y^2 + z^2 * 1] \wedge [x > 0] \wedge [y > 0] \wedge [z > 0]\right], \quad * \in \{=, \neq, <, >, \leq, \geq\}.$$

$$\left\{\begin{array}{l}\left\{\begin{array}{l}\left\{\begin{array}{llll} cell & 0 < z < \sqrt{1-x^2-y^2} & & \\ cell & z = \sqrt{1-x^2-y^2} & 0 < y < \sqrt{1-x^2} & \\ cell & z > \sqrt{1-x^2-y^2} & & 0 < x < 1 \end{array}\right. \\ \left\{\begin{array}{llll} cell & z > 0 & y = \sqrt{1-x^2} & \\ cell & z > 0 & y > \sqrt{1-x^2} & \end{array}\right. \end{array}\right. \\ \left\{\begin{array}{llll} cell & z > 0 & y > 0 & x = 1 \\ cell & z > 0 & y > 0 & x > 1 \end{array}\right. \end{array}\right.$$

Figure 4.4: The inequality sub-CAD for Example 4.8 in Maple's piecewise output format.

We know that constructing a complete CAD will contain 135 cells. If we utilise all three inequalities it is possible to only return 7 cells.

The sub-CAD of $\mathbb{R}^1$ is the same as in Example 4.7, however the subsequent lifting steps offer further savings:

- **1-D sub-CAD:** 7 cells are reduced to 3 cells (Example 4.7: $7 \to 3$);
- **2-D sub-CAD:** 13 cells are reduced to 5 cells (Example 4.7: $33 \to 13$);
- **3-D sub-CAD:** 31 cells are reduced to 7 cells (Example 4.7: $135 \to 51$).

The final inequality sub-CAD that would be produced is shown in Figure 4.4, in Maple's piecewise output format.

Constructing a Partial CAD would include at least a further 20 cells, namely:

- The 4 cells that are $\{x = 0, -1 < x < 0, x = -1, x < -1\} \times \mathbb{R}^2$;
- The 4 cells that are $0 < x < 1 \times \{y < -\sqrt{1-x^2}, y = -\sqrt{1-x^2}, -\sqrt{1-x^2} < y < 0, y = 0\} \times \mathbb{R}$;
- The 4 cells that are $0 < x < 1 \times 0 < y < \sqrt{1-x^2} \times \{z = 0, -\sqrt{1-x^2-y^2} < z < 0, z = -\sqrt{1-x^2-y^2}, z < -\sqrt{1-x^2-y^2}\}$;
- The 2 cells that are $x = 1 \times \{y < 0, y = 0\} \times \mathbb{R}$;
- The 2 cells that are $x = 1 \times y > 0 \times \{z < 0, z = 0\}$; and
- The 2 cells that are $x > 1 \times \{y = 0, y < 0\} \times \mathbb{R}$;
- The 2 cells that are $x > 1 \times y > 0 \times \{z < 0, z = 0\}$.

To this end, an inequality sub-CAD offers direct savings over a partial CAD.

There is a chance that identification of algebraic numbers involved in non-trivial inequalities (for example nested algebraic numbers) could prove costly to identify the valid regions defined by inequalities. However we can construct a 1-layered inequality sub-CAD with little effort as all sample points involved can be chosen in $\mathbb{Q}$.

Along with 1-layered sub-CADs, we could combine inequality sub-CADs with various other ideas from sub-CADs in obvious ways. For example, if the sphere in Example 4.8 was an equational constraint, then producing a variety inequality sub-CAD would restrict the output shown in Figure 4.4 to the single cell defining the surface of the strictly positive octant of the sphere.

Ideally we would wish to incorporate these simple inequalities into the projection stage as well as the lifting stage. Work on generic projection in partial CAD [SS03] appeals to assumptions in the parameters of the input to simplify projection and could hopefully be combined with this lifting process. There is also scope for simpler well-orientedness conditions: a projection operator may fail a well-orientedness condition outside of the domain and so the output is still correct.

Without a full implementation we cannot run any significant experimentation, but it seems clear that inequality sub-CADs could provide substantial savings in cells and timing.

4.7.2 Further Extensions

There are a many other possible ways to extend the sub-CAD work and we list a few possibilities.

When detailing algorithms for layered and variety sub-CADs, certain restrictions on permissible inputs are imposed. It would obviously be advantageous to extend the application of these algorithms to treat equational constraints of low level or that define varieties with co-dimension greater than 1. The restriction of layered variety sub-CADs to LV-well-oriented (Definition 4.5) input is to avoid cases, such as the Whitney Umbrella, where lifting to the variety increases dimension (and so Lemma 4.6 does not hold). Taking care of this degeneracy would increase the power of this algorithm.

Along with a selection of sub-CADs, examples have also been given of where they may be applicable. Identifying general classes of problems where a given sub-CAD is sufficient will extend the benefit of the theory and offer more practical uses for sub-CAD.

Section 4.1.1 gave a collection of existing CAD techniques (such as partial CAD) that can be adapted to construct sub-CADs, and these should be investigated.

Clearly, there are possible definitions for other types of sub-CADs and algorithms to construct them. Along with the idea of utilising simple inequalities in Section 4.7.1, it may be possible to construct sub-CADs with respect to other common properties of CAD problems (pairs of related constraints, certain block structures of quantifiers, other logical connectives such as implication).

In Section 3.8 it was suggested that, when constructing a TTICAD, lifting could be done only with respect to formulae that are appropriate for that cell. This can be thought of as an analogue of partial CAD for TTICADs and could be combined with sub-CAD ideas to only output cells that are relevant to the problem.

All the current work on sub-CADs has been developed in relation to the projection and lifting construction method for CAD. An obvious extension would be to consider how to produce layered and variety sub-CADs for the regular chains algorithms. It may be possible to restrict the complex decomposition before converting to a CAD, offering large savings. It is not obvious whether a recursive layered algorithm would be possible with this method.

An application of sub-CADs within heuristics for formulating a CAD problem is given in Section 5.4.4, and an application of sub-CADs to the reformulation of a notable problem in CAD theory is given in Section 6.3.9. Finally, a discussion of how adjacency may interact with sub-CADs is discussed in Appendix A.

4.8 Solotareff-3

We consider again the Solotareff-3 problem given in Section 2.12.

$$(\exists\, u)(\exists v)\Big[[3v^2 - 2v - a = 0] \ \wedge\ [v^3 - v^2 - av - 2b + a - 2 = 0] \\ \wedge\ [3u^2 - 2u - a = 0] \ \wedge\ [u^3 - u^2 - au - a + 2 = 0] \ \wedge\ [1 \leq 4a] \ \wedge\ [4a \leq 7] \\ \wedge\ [-3 \leq 4b] \ \wedge\ [4b \leq 3] \ \wedge\ [-1 \leq v] \ \wedge\ [v \leq 0] \ \wedge\ [0 \leq u] \ \wedge\ [u \leq 1]\Big]. \quad (4.21)$$

Tables 4.2 and 4.3 detail the results of a collection of sub-CAD techniques.

As there are four equational constraints present in (4.21) then we can certainly attempt to build a variety sub-CAD. As with building an equational constraint CAD, using either of the first two constraints results in theoretical failure due to nullification. Constructing a variety sub-CAD with the third or fourth equational constraint proves efficient, with the third performing particularly well. This can offer a saving of up to 84.8% and 88.1% over a sign-invariant CAD for the two orderings, and savings of 60.3%

Technique	Cells	Time	Section	Page
PL-CAD (Col)	54037	255.304	2.3	30
PL-CAD (McC)	54037	266.334	2.3	30
EC-CAD (f_3)	20593	65.856	2.4.4	40
EC-CAD (f_4)	22109	102.781	2.4.4	40
V-CAD (f_3)	8195	63.387	4.2	114
V-CAD (f_4)	8953	95.233	4.2	114
1-L-CAD	5012	5.944	4.3	119
2-L-CAD	21426	133.245	4.3	119
3-L-CAD	41333	318.657	4.3	119
4-L-CAD	51947	354.313	4.3	119
5-L-CAD	54037	428.707	4.3	119
1-LV-CAD (f_3)	1372	3.222	4.4	128
2-LV-CAD (f_3)	4754	43.265	4.4	128
3-LV-CAD (f_3)	7480	92.708	4.4	128
4-LV-CAD (f_3)	8195	113.340	4.4	128
1-LV-CAD (f_4)	1522	4.347	4.4	128
2-LV-CAD (f_4)	5229	72.075	4.4	128
3-LV-CAD (f_4)	8185	136.119	4.4	128
4-LV-CAD (f_4)	8953	157.836	4.4	128

Table 4.2: The Solotareff-3 problem with sub-CAD techniques — variable order $a \prec b \prec v \prec u$.

and 60.5% over an equational constraint CAD. Any of the variety sub-CADs are sufficient to solve the problem.

As there is only a a single solution to the problem, a layered sub-CAD is not appropriate to solve the problem. At most, a 4-layered sub-CAD could be used to show that there is a finite number of possible solutions. However, to demonstrate the power of the sub-CAD theory we compute all possible layered sub-CADs. We can see that computing a 1-layered sub-CAD is very efficient, due to the lack of algebraic numbers, and produces a proportionally small amount of cells. It is interesting to note that the size of the 1-layered sub-CADs suggest that $a \prec b \prec v \prec u$ is the optimal order (which is indeed the case) and this will be investigated as a general heuristic in Section 5.4.

We can also construct layered variety sub-CADs which offer further substantial savings. We can only construct four layers, as the variety is of co-dimension 1, and each level produces a cell saving over the layered sub-CAD. A 1-layered variety sub-CAD offers the largest cell savings, 97.5% and 98.1% for the two variable orderings, along with savings of 98.8% and 99.3% in construction time compared to the complete CADs.

Finally, we note that in the presence of simple inequalities for every variable, the work discussed in Section 4.7.1 should be applicable, at least in the base variable when

Technique	Cells	Time	Section	Page
PL-CAD (Col)	161317	916.105	2.3	30
PL-CAD (McC)	154527	857.357	2.3	30
EC-CAD (f_3)	48475	175.139	2.4.4	40
EC-CAD (f_4)	63583	324.663	2.4.4	40
V-CAD (f_3)	19127	173.083	4.2	114
V-CAD (f_4)	25563	295.556	4.2	114
1-L-CAD	13716	17.868	4.3	119
2-L-CAD	59598	516.734	4.3	119
3-L-CAD	116924	1689.886	4.3	119
4-L-CAD	148205	2925.458	4.3	119
5-L-CAD	154527	4876.479	4.3	119
1-LV-CAD (f_3)	3040	6.153	4.4	128
2-LV-CAD (f_3)	10808	76.251	4.4	128
3-LV-CAD (f_3)	17332	155.035	4.4	128
4-LV-CAD (f_3)	19127	178.588	4.4	128
1-LV-CAD (f_4)	4132	9.043	4.4	128
2-LV-CAD (f_4)	14560	139.543	4.4	128
3-LV-CAD (f_4)	23211	282.426	4.4	128
4-LV-CAD (f_4)	25563	322.241	4.4	128

Table 4.3: The Solotareff-3 problem with sub-CAD techniques — variable order $b \prec a \prec v \prec u$.

decomposing $\mathbb{R}^1$.

4.9 Conclusion

In this chapter we introduced and formalised the idea of a cylindrical algebraic sub-decomposition (sub-CAD), which is a subset of a CAD. Highlighting related ideas in the literature, it is clear that a sub-CAD is of great use in many applications of CAD technology to a given problem. Two new sub-CADs were introduced: variety sub-CADs and layered sub-CADs. Algorithms were given for both types of sub-CAD, and a recursive algorithm for layered sub-CADs was also provided. All algorithms were proven correct and examples given to demonstrate their effectiveness. It was discussed how these can be combined to form layered variety sub-CADs, and how these concepts interact with the TTICAD theory of Chapter 3 to form sub-TTICADs.

Complexity analysis of variety sub-CADs and 1-layered variety sub-CADs showed the formal benefit of the new theory, and this was supported by experimental results indicating where sub-CADs offer startling improvements in efficiency. Finally, extensions of the sub-CAD theory were proposed.

Chapter 5

Formulating Problems for CAD

Before constructing a CAD, many decisions have to be made to formulate a problem into a suitable form. One of these factors that has been studied is the effect of variable ordering in the complexity of CAD [BD07, DSS04] but other factors include the separation of sub-formulae and choice of equational constraints.

It is possible to use various heuristics to make informed choices for these factors in formulation. We evaluate the use of existing heuristics and introduce new metrics and heuristics. We present promising results for using machine learning to decide the best variable ordering for a problem, and planned research will extend this to other decisions. We also use ideas from Chapter 4 to inspire a new heuristic.

Author's Contribution and Publication

The work in Section 5.2 was collaborative work with the rest of the Bath research group: the author was involved in all discussions and experimentation, but the new heuristic (`ndrr`) was invented by another researcher. The work in Section 5.3 was collaborative with a research group at the University of Cambridge: the author began the collaboration with Huang and, together, designed the experiments and feature list. The author helped prepare the experiment, which was conducted by Huang, and discussed the results. The work in Section 5.4 is the author's.

The work from Section 5.2 has been published in [BDEW13, EBC+14, EBDW14]. The work in Section 5.3 will be published in [HEW+14b, HEW+14a]. The work in Section 5.4 was initially discussed in the technical report [WE13] and has been submitted to [WEBD14].

5.1 Issues when Formulating a Problem for CAD

Given a problem for which we wish to construct a CAD there are a number of choices that are necessary to make before a CAD algorithm can be used. When provided with either a Boolean formula (which may or may not be quantified) or a set of polynomials (which may or may not be given with equational conditions), we refer to the process of creating a complete input for a CAD algorithm as the **formulation** of the problem.

When formulating a problem the choices that need to be made vary depending on which algorithm is to be used. These choices may include:

- **variable ordering:** for any CAD algorithm a variable ordering must be chosen (that is compatible with any quantification);
- **equational constraint designation:** for any CAD algorithm involving equational constraints, there may be a choice of which to designate;
- **formulae decomposition:** for TTICAD algorithms there may be a choice of ways to decompose the formula into sub-formulae;
- **input ordering:** for incremental algorithms, there may be a choice of the order of input.

Previous work [DSS04, Bro04, BD07] has looked at the effect of variable ordering on the complexity of the CAD constructed, and suggested various heuristics (discussed in Section 2.6.3). Little has been discussed in literature regarding the other decisions needed to formulate a problem for CAD (although presumably CAD users have developed their own intuition for these choices) and this chapter discusses methods for deciding these.

5.2 Heuristics for Formulation

We now discuss each of the points raised in Section 5.1, identifying metrics and heuristics that can be used to help make a near-optimal choice.

Due to the nature of the work, this section will be necessarily experimental and speculative. All the following work was presented and published in [BDEW13, EBC+14, EBDW14]. The author was involved in the discussions and experimentation for the paper; however the new heuristics were created by another member of the research group. Therefore we give only a survey of the results.

5.2.1 Variable Ordering

Section 2.6.3 discussed the work of [DSS04] and [Bro04] in developing heuristics for selecting a variable ordering for a given CAD problem. In particular, they suggest the following two heuristics:

- **Sum of Total Degree [DSS04]** For each variable ordering compute the full projection set, then select the ordering that produces the production set with smallest `sotd` (the **sum of total degrees** of all monomials in the set). The variable order can also be selected greedily by projecting once and minimising `sotd`, then repeating for all projection steps.

- **Brown Heuristic [Bro04]** decides variable ordering with following criteria (breaking ties with successive criteria):

  1. Project the variable with the lowest overall degree in the input;
  2. Project the variable with the lowest maximum total degree of all monomials in which it occurs;
  3. Project the variable with the smallest number of monomials in the input which contain the variable.

  If there is still a tie after utilising all three criteria then a decision is made lexicographically[1].

Both Brown's heuristic and `sotd` can be deceived by problems with intricate complex geometry that does not translate into $\mathbb{R}^n$ [BDEW13]. To try and encapsulate the real geometry of the problem (which is what influences the CAD) we define a new metric: `ndrr`.

Definition 5.1 ([BDEW13])**.**
Let F be a set of polynomials. For a given variable ordering `x` we compute the full projection set (with respect to a given ordering) and define the **number of distinct real roots** metric, denoted `ndrr`, to be the number of distinct real roots of univariate projection polynomials.

This metric is designed to capture the complexity of the one-dimensional CAD, which has a bearing on the complexity of the complete CAD. The associated heuristic is to choose the variable ordering with the minimal `ndrr` value.

[1]The lexicographic choice is made with respect to the system being used: Maple and Qepcad will behave differently due to their respective variable ordering conventions.

It was demonstrated in [BDEW13], that `ndrr` can cope with problems that trick the alternative heuristics, but can also be deceived itself (such as deciding the positive semidefiniteness of the general quartic).

There are some very clear detriments to using `ndrr` as a heuristic. The cost of computing `ndrr` can be great and is equivalent to constructing the base CAD of $\mathbb{R}^1$. In his complexity analysis of CAD ([Col75], discussed in Section 4.5), Collins states that using Heindel's algorithm real root isolation can be of the order $d^8 + d^7l^3$ for a single polynomial with degree d and norm length l. Considering the potential increase in degree and number of polynomials through the projection operator, the complexity of constructing a one-dimensional CAD using Collins' operator for a set of m polynomials in n variables with degree d and max norm length l is given in [Col75] as:

$$(2d)^{3^{n+3}} m^{2^{n+2}} l^3.$$

Although the use of improved projection operators will simplify this slightly, the base case will always remain doubly exponential (as demonstrated in [Dav86]).

In [DSS04] the authors avoided computing `sotd` for all $n!$ variable orderings by considering a greedy algorithm, where the next projection variable was chosen by doing a single projection with respect to all valid variables and computing `sotd` of the partial projection set. This reduces the number of individual projection computations from $(n-1)\cdot n!$ to $n(n+1)/2$. There is no obvious way to adapt `ndrr` into a greedy algorithm and so all variable orderings need to be projected fully to make a comparison of the orderings.

As `ndrr` has both strong benefits and shortcomings, [BDEW13] suggests its use alongside `sotd` (or another heuristic) by either using one heuristic to break ties or by taking a weighted combination of the two metrics. Due to the relative costliness of `ndrr` and the historical precedent of `sotd`, it seems prudent to use `sotd` as the primary heuristic, breaking ties with `ndrr`. Using this combination of `sotd` and `ndrr` would correctly identify the optimal variable ordering for the deceptive examples mentioned above.

Coupled Variables

In [Phi11] it was noted that `sotd` and Brown can struggle to distinguish between variables that are the real and imaginary parts of a complex variable, which we call **coupled variables**. When analysing complex formulae with CAD, it is necessary to describe the branch cuts of the formula in real space and, by construction, coupled variables become

hard to distinguish from degree alone. However, the ordering of couple variables can be important, and `ndrr` can be used to distinguish these as shown in the following example.

5.2.2 Equational Constraint Designation

Assuming that a variable ordering has been chosen, to formulate a problem for CAD utilising equational constraints by projection and lifting requires the identification of a single equational constraint to project with respect to. We call such an equational constraint, the **designated equational constraint** for the problem.

The choice of which equational constraint to designate can have a substantial effect on the complexity of the resulting CAD. We are restricting our projection to when polynomials interact with the variety defined by the equational constraint, so we would ideally like to select the equational constraint that interacts least with the other polynomials.

The metrics `sotd` and `ndrr` were used to try and measure this interaction. The metrics `S` and `N` were defined to be the `sotd` and `ndrr`, respectively, of the appropriate full projection set: the equational constraint projection set, ${}_{\mathbf{M}}\mathbf{P}_E(A)$, followed by applications of the McCallum projection operator, ${}_{\mathbf{M}}\mathbf{P}$.

Remark 5.1.
It is not possible to apply Brown's heuristic directly to equational constraint designation. It would be interesting to do further investigation on whether the heuristic can be adapted to this problem: the underlying ideas of minimising degrees of polynomials, degrees of monomials, and number of monomials could be transferred onto different sets of polynomials derived from the equational constraint.

The results from [BDEW13] demonstrated `S` and `N` are useful, but that it is not simple to select an optimal equational constraint designation. In all examples but one the optimal designation with respect to cell count and time is a designation with the lowest value of `S` and `N`. However, there are examples where `S` or `N` struggle individually.

The results demonstrated that selecting an optimal equational constraint to designate is important. In particular, they illustrated that the choice can not only provide cell savings but also affect the validity of the equational constraint projection operator. The `S` and `N` heuristics do a fair job of predicting good designation, although both can be tricked (see [BDEW13, Example 5]). This is an area where further research could provide new heuristics.

Remark 5.2.
The issue of equational constraint designation is not present when using the Regular

Chains incremental CAD. It is possible to utilise all equational constraints when constructing a CAD (see, for example, Table 6.9 in Section 6.2.8) and so designation is not necessary.

5.2.3 Formulation for TTICAD

When using the projection and lifting TTICAD algorithms from Chapter 3, the input needs to be a list of quantifier-free formulae.

As in Section 5.2.2, if any of these formulae have more than one equational constraint then one needs to be designated for use with the projection operator. This decision can be assisted with the use of the metrics `sotd` and `ndrr` by constructing the full projection sets with each possible combinations of designated equational constraints and selecting the designations that minimise the metrics.

It is also possible, in certain cases, to decompose Φ into sub-formulae in different ways. For example, a formula can be separated into subformulae, or formulae with the same equational constraint can be combined. This can also have an effect on the complexity of the CAD [BDEW13].

Unfortunately `sotd` and `ndrr` are not completely accurate in predicting an optimal decomposition [BDEW13]. This is unsurprising as the splitting of formulae can be very subtle. It is not clear whether `sotd` or `ndrr` is the most appropriate so a hybrid approach is sensible.

Splitting or joining of formulae consisting of pure conjunctions is straightforward. If two formulae are connected by a disjunction then it is possible to join them if they share an equational constraint (which would become the designated equational constraint in the new formula). For example $[f = 0 \wedge g > 0] \vee [f = 0 \wedge h > 0]$ can be joined to become $[f = 0 \wedge [g > 0 \vee h > 0]]$. It is clear from the TTICAD projection operator that such a joining would not affect the TTICAD construction and so is not an issue within formulation.

The number of potential ways to decompose a formula Φ and designate equational constraints soon becomes combinatorially huge. Therefore it was proposed in [BDEW13] to formulate a problem Φ in the following manner, treating each subformulae in turn:

1. Put the formula into disjunctive normal form: $\bigvee_i \varphi_i$ so that each φ_i is a conjunction of atomic formulae.

2. For each φ_i let m_i be the number of equational constraints:

- **If $m_i = 0$:** then there is no choice for designation (and Algorithm 3.2 will need to be used to accommodate this).
- **If $m_i = 1$:** then the sole equational constraint should be designated.
- **If $m_i > 1$:** then we consider all possible partitions of the formula φ_i into subformulae with at least one equational constraint in each, and all the different equational constraint designations within those subformulae with more than one. Choose the partition which minimises a chosen metric (`sotd` or `ndrr`).

3. Let $\hat{\Phi}$ be the list of the new formulae and use this for input to the TTICAD algorithm.

This will not always provide the optimal formulationand will depend on the choice of metric used. However, it provides a practical and implementable way to formulate a problem for TTICAD.

5.2.4 Incremental Algorithms

The formulation ideas for projection and lifting CAD algorithms do not automatically apply to regular chains algorithm, and the incremental algorithms have their own choices.

In [EBC+14] it is first noted that it is sensible to process equational constraints first, and all equational constraints within a single formula together. This is both logical and practical: the constraints offer greater benefit by being considered before any non-equational constraints, and by considering all the equational constraints in a formula before considering the next formula we can avoid unnecessary identification of shared roots.

It was then shown that whilst the incremental regular chains TTICAD algorithm can make use of all equational constraints in each formula, the order the equational constraints are considered can make a difference to the efficiency. Further, the order the formulae are considered is also important.

The reason for this difference is due to the incremental construction of the complex cylindrical tree (whilst maintaining the regular chain structure). It is important to understand this behaviour and develop a heuristic to make an optimal choices. To do this the following proposition and definition were given with respect to the `RC-TTICAD` algorithm.

Proposition 5.1 ([EBC+14])**.**
The output of `RC-TTICAD` *is always sign-invariant with respect to the discriminant of the first equational constraint in each formula.*

The output of `RC-TTICAD` *is always sign-invariant with respect to the cross-resultants of the first equational constraints in each formula.*

Definition 5.2 ([EBC+14])**.**
For a given constraint ordering $\mathtt{o}$, let P be the set of equational constraints which are ordered first in each formula. Define the **constraint ordering set**, $\mathcal{C}_{\mathtt{o}}$ as the discriminants and cross resultants in the main variable of the ordering.

$$\mathcal{C}_{\mathtt{o}} := \left(\bigcup_{p \in P} \{\text{disc}_{x_n}(p)\} \right) \cup \left(\bigcup_{\substack{p,q \in P \\ p \neq q}} \{\text{res}_{x_n}(p,q)\} \right).$$

Comparing the `sotd` of the constraint ordering sets proves ineffective, whilst their total degree proves to be more effective at distinguishing an optimal ordering. This is unsurprising considering that the latter concerns the complex geometry of the problem (which is featured in the complex cylindrical tree of an regular chains TTICAD) whilst the former encodes the sparseness of the polynomials (which is more important when using a projection operator). This prompts the following heuristic.

Definition 5.3 ([EBC+14])**.**
Define the **EC ordering heuristic** as selecting the first equational constraint to be processed in each formula such the corresponding constraint ordering set has lowest sum of degrees of the polynomials within (all taken in the second variable of the ordering).

Utilising the EC ordering heuristic (breaking ties with either `sotd` or `ndrr`) proves effective at ordering equational constraints within each formula, but cannot help decide the order to consider each formula.

It is best to place a formula with only a single equational constraint first (or indeed a formula with no equational constraints). After which we use the following heuristic.

Definition 5.4 ([EBC+14])**.**
Define the **CCD size heuristic** as selecting a constraint ordering by constructing the complex cylindrical decomposition for each, extracting the set of polynomials used in each tree, and choosing the one to refine to a CAD whose set has the lowest sum of degree of the polynomial within (each taken in the main variable of that polynomial).

This combines with the EC ordering heuristic to form a hybrid heuristic.

Definition 5.5 ([EBC+14])**.**
Define the **constraint ordering heuristic** as using the EC ordering heuristic to suggest

the best subset of constraint orderings and then having the CCD size heuristic to pick from these, splitting any further ties by picking lexicographically.

Through systematic testing of the three heuristics (on 100 randomly constructed examples) it is shown that the CCD size heuristic generally performs better than the EC ordering heuristic at picking the smallest TTICAD, but does so at a much greater cost. This is to be expected, but the degree of correlation of the CCD size heuristic proves that the complex and real decompositions are very closely linked.

The hybrid constraint ordering heuristic offers significantly more savings than the EC ordering heuristics and takes significantly less time than the CCD size heuristic. This therefore seems to be a good multi-purpose approach: using the EC ordering heuristic if the speed of the heuristic is a priority or the CCD size heuristic if a low cell count is of a priority.

It is also noted in [EBC+14] that two formulation issues with projection and lifting TTICAD do not apply to regular chains. It is not necessary to designate a single equational constraint (although selecting an order for the equational constraints is a similar choice) as the incremental algorithm can utilise all constraints in the formulae. The sophistication of the incremental regular chains TTICAD also renders the option to decompose formulae further, as detailed in Section 5.2.3, obsolete: decomposing a formula into extraneous sub-formulae will always give a higher cell count with regular chains TTICAD.

In [EBDW14] the issue of selecting a variable ordering was considered with respect to the regular chains TTICAD algorithm. Along with Brown's heuristic, `sotd`, and `ndrr`, the heuristic used in the `RegularChains` heuristic command `SuggestVariableOrder` (which is used for all their decomposition commands, including `CylindricalAlgebraicDecompose`).

Definition 5.6 (`RegularChains[SuggestVariableOrder]`).
The **triangular heuristic** uses the following list of criteria to decide the variable order, breaking ties with successive criteria:

1. Let $v^{[1]} = \max(\{\deg(f, v) \mid f \in P\})$ and let $x \prec y$ if $x^{[1]} > y^{[1]}$.
2. Let $v^{[2]} = \max(\{\text{tdeg}(\text{init}(f, v)) \mid f \in P \text{ (containing } v)\})$ and let $x \prec y$ if $x^{[2]} > y^{[2]}$.
3. Let $v^{[3]} = \sum_{f \in P} \deg(f, v)$ and let $x \prec y$ if $x^{[3]} > y^{[3]}$.

Note that the first step is identical to the Brown heuristic and the second step is similar (the Brown heuristic considers the maximal total degree of any monomial containing v, not just the leading coefficients).

To evaluate the performance of the heuristics, six categories of random examples were considered with varying numbers of equational constraints. Of the four original heuristics, `sotd` offers the greatest cell savings but the cost of this heuristic means that the Brown heuristic is the most time efficient. Hybrid heuristics combining `sotd` and `ndrr` are more effective, but Brown is still more efficient with respect to overall time. Applying `sotd` and `ndrr` to the TTICAD projection set offers larger savings in both cell count and overall time, even though RC-TTICAD does not involve projection.

Finally, a new heuristic is given, based on the constraint ordering set (Definition 5.2). This offers near-maximal cell savings along with the greatest net time savings.

5.3 Applying Machine Learning to CAD

Whilst both relatively modern advances in computer science, there has been little interaction between symbolic computation and machine learning. This is, perhaps, due to it being difficult to find an appropriate question for machine learning to consider, and the additional restriction that this question has to be accompanied by a large enough data bank of feasible problems for it to work on. Working in collaboration with researchers at the University of Cambridge this appears to be the first published work on an application of machine learning to problem formulation for computer algebra (although there have been recent applications to automated theorem proving [HP13]).

The work in this section follows [HEW+14b]. The initial collaboration was between the author and Zongyan Huang of the University of Cambridge, and once a potential application of machine learning within CAD was identified the two research groups started a formal collaboration. The experiments were designed by the author, Huang, and England; the experiments were conducted by Huang, with assistance from the author and England in providing scripts to format the examples, compute the features in Maple, and construct the CADs in Qepcad; the results were analysed and discussed by both research groups.

We will apply machine learning to the problem of choosing variable ordering for a CAD problem. It is not appropriate to choose a variable ordering directly with machine learning, for reasons discussed later in this section, and so we instead choose a heuristic with machine learning (which then selects a variable ordering).

5.3.1 Background on Machine Learning

We first give a brief description of machine learning and the particular technique used: support vector machines. This is given in further detail in [HEW+14b].

Machine learning encompasses programs that can take a collection of data and infer rules that can then be used to classify or optimise the treatment of further data. There are many machine learning techniques and algorithms available, and we will consider a recent invention: the **support vector machine** (**SVM**) [STV04]. This a machine learning technique well-suited to efficiently deal with high-dimensional data and can cope with diverse sources of data.

To use an SVM a vector of features must be created for each piece of data. The idea is to then use the vectors of the training data to compute a hyperplane that can be used to predict the classification of new data based on their feature vector. An SVM can use a kernel function to map data into a kernel-defined feature space and computes inner products between all pairs of data vectors. This avoids the computation of coordinates of data and is generally cheaper than explicit computation.

Once a SVM has been initialised there are two stages: learning and classifying. In the learning phase the model parameters are set based on the training data, parameter choices, and the kernel function. The classification stage then constructs a hyperplane of co-dimension 1 in the feature space according to the model, which divides the space into two distinct classes. A new feature vector can then be classified with respect to this hyperplane with the distance to the hyperplane representing the confidence in the prediction.

Previous Work

Recently [HP13] the research group at Cambridge have looked at applying machine learning techniques to decision procedures for the theory of real closed fields. Using the SVMs they consider choosing the most efficient real closed fields decision procedure for the MetiTarski software [AP08] choosing between Z3, Mathematica and Qepcad.

With a data set of 825 problems, 418 were used as a learning set. A further 213 problems were used to validate and decide kernel options. This left 194 problems to test the effectiveness of the machine learning technique. The efficiency was measured by considering the number of problems proven by MetiTarski with a given decision procedure. The results are:

- Z3: 160 problems proven;

- MATHEMATICA: 153 problems proven;
- QEPCAD: 158 problems proven;
- Machine Learning: 163 problems proven.

It can be seen that using the Machine Learning techniques is beneficial. As a benchmark, choosing the best decision procedure would prove 172 out of the 194 test problems, giving SVM as a 94.7% optimal choice.

Although a small data set, this proves that machine learning can be useful in the theory of real closed fields and motivates our investigation into its application to CAD.

5.3.2 Design of Experiment

We have seen that variable ordering is a key choice in formulating a CAD problem and can prove the difference between a doubly exponential or constant number of cells [BD07]. Unfortunately we cannot apply machine learning to directly select an optimal variable ordering for a problem. In essence, a SVM cannot distinguish between variable ordering choices: it considers all variable orderings to be essentially the same (simply a choice) and so cannot consider relationships between the orderings or associate a feature relating to a variable with the variable's position within an order. It therefore loses the meaning behind the orderings. Instead, we use machine learning to select a heuristic (to then select a variable ordering) which allows the heuristics to encode the relationships of the variables and orderings.

Heuristic Choices

In Section 5.2 we discussed three heuristics that can be used to choose a variable ordering: `sotd`, `ndrr`, and Brown's heuristic (in the case that any heuristic identifies more than one variable ordering as a suitable choice, the first of the choices lexicographically[2] is selected). Machine learning was used to select between these three heuristics.

All the heuristics were computed within MAPLE using commands from the `ProjectionCAD` package. QEPCAD was used to compute the CADs for two reasons: it is a heavily optimised and freely-available implementation of projection based CAD; and it allows us to compare problems for CAD that are both quantified and unquantified.

[2]This lexicographic choice changes for QEPCAD and MAPLE due to their variable ordering conventions. We select with respect to MAPLE, but this choice is arbitrary and the important point is that it is consistent and reproducible.

Data Set

Any application of machine learning requires a substantial problem set to allow for enough data to split into sizeable training and evaluation sets. Therefore, the NLSAT database[3] [New12] was used and adapted for use with CAD.

The problems from the NLSAT database with three variables, totalling 7001 examples, were used. This variable restriction avoided the possibility of errors relating to well-orientedness of the McCallum projection. The NLSAT database is a collection of quantifier elimination problems and we considered each example in two manners: quantified and unquantified.

- **Quantified:** The problems are fully existentially quantified. We give this quantified version to QEPCAD and use the `d-stat` command following construction to obtain the number of cells constructed in the partial CAD.
- **Unquantified:** Removing the existential quantifiers, each problem gives a formula to construct a CAD of $\mathbb{R}^3$ with respect to. Then `d-fpc-stat` is used to compute the number of cells produced in the CAD of $\mathbb{R}^3$.

Sample QEPCAD input for quantified and unquantified examples is given in Section C.3.

Remark 5.3.
CAD is generally not the optimal method for solving a SAT problem (see for example [JdM12]). The use of the existential problems is due to the data set rather than it being a requirement of the technology. An advantage to this choice is that a fully existential or fully universal quantification allows for all six possible variable orderings. Further work will include expanding the experiments to consider other forms of quantification.

The examples from the NLSAT database were randomly split into three sets: 3545 problems in the training set, 1735 problems in the validation set, and 1721 problems in the test set[4].

Feature Set

When using a SVM a vector of features needs to be provided for all problems. These features are not pre-determined and should be chosen to highlight, numerically, any

[3] Available online at: `http://cs.nyu.edu/~dejan/nonlinear/`.
[4] All data used for the experiment is available for download at `http://www.cl.cam.ac.uk/~zh242/data`.

Feature	Description
1	Number of polynomials.
2	Maximum total degree of polynomials.
3-5	Maximum degree of x_0, x_1, x_2 among all polynomials.
6-9	Proportion of x_0, x_1, x_2 occurring in polynomials.
9-11	Proportion of x_0, x_1, x_2 occurring in monomials.

Table 5.1: The feature vector computed for all examples. The proportion of a variable occurring in polynomials/monomials is the number of polynomials/monomials that variable occurs in divided by the total number of polynomials/monomials.

properties of the input that may be relevant to the heuristic choice and the CAD produced. Eleven features were identified for the examples, with respect the variable labels (x_0, x_1, x_2), and they are given in Table 5.1.

All the features used are trivial to compute and are properties of simply the input (not requiring any computation or projection). The number of features is smaller than in many machine learning experiments: other features were considered (such as the size of coefficients and proportion of constraints that are equations) but were found to not provide any benefit. Identifying other useful features to improve the performance of machine learning is a potential area for future investigation.

The feature vector was computed within Maple using simple commands such as `degree` and `nops` (the number of operands of an expression, which gives the size of a set). The conversion from Nlsat to Maple for this computation is described in Section C.3.

Once the feature vectors had been calculated for the 3545 elements of the training data, each feature was normalised to have zero mean and unit variance. This normalisation was then applied to the validation and test sets.

Evaluation of Heuristic Choices

For each problem there are six permissible variable orderings and Qepcad was used to build a CAD for all of these orderings. The number of cells was measured, in the appropriate manner, in every case. Cell counts and timing are usually closely positively correlated (this will also be shown in Figure 6.1) so the experimentation can also be used for selecting an ordering for near-optimal construction time.

All three heuristics (Brown, `sotd`, `ndrr`) were computed within Maple (using commands from the `ProjectionCAD` module and the scripts discussed in Section C.3) and for each example the ordering suggested by each heuristic was recorded, along with the

cell count from QEPCAD for that ordering. We will use the following definitions related to variable orderings and heuristics.

Definition 5.7.
For a given example the **best variable ordering** is defined to be the variable ordering resulting in the smallest cell count. If multiple orderings produce the minimal number of cells then they are all considered best variable orderings.

For a given example the **optimal variable ordering** with respect to the three heuristics (Brown, `sotd`, `ndrr`) is defined to be the variable ordering with the lowest cell count out of those orderings selected by the heuristics. If multiple orderings selected by the heuristics produce the minimal number of cells (of those chosen by the heuristics) then they are all considered optimal variable orderings. We say that a heuristic is an **optimal heuristic** if it selects an optimal variable ordering.

Machine learning was used to predict an optimal heuristic, and therefore produce an optimal variable ordering. It is of course possible that the optimal and best variable orderings can be different.

Each feature vector in the training set has an associated label for each heuristic: $+1$ for positive examples where the heuristic in question selected an optimal variable ordering; -1 for negative examples where the heuristic in question did not select an optimal variable ordering. These labels are then used by the SVM to decompose the feature vector space and enable it to predict heuristic choice. The parameter choices for the SVM were chosen methodically, as detailed in [HEW+14b].

5.3.3 Results of experimentation

For each heuristic, the number of problems for which an optimal variable ordering was chosen is used as a measure of its efficacy. For machine learning, we use the number of problems of which it selected an optimal heuristic as a measure of its efficacy.

Table 5.2 details the results. There are 13 possible[5], mutually exclusive, cases depending on whether each heuristic selected an optimal variable ordering and whether machine learning selected an optimal heuristic. For each heuristic a Y indicates that heuristic selected an optimal variable ordering, and a N indicates it did not. For the machine learning column a Y indicates it selected an optimal heuristic, and a N indicates it did not.

[5]Of the 16 possible cases, at least one heuristic must be optimal (removing two cases) and if all heuristics are optimal then machine learning is always successful (removing one case).

Case	Machine Learning	`sotd`	`ndrr`	Brown	Quantifier-Free	Quantified
1	Y	Y	Y	Y	399	573
2	Y	Y	Y	N	146	96
3	N	Y	Y	N	39	24
4	Y	Y	N	Y	208	232
5	N	Y	N	Y	35	43
6	Y	N	Y	Y	64	57
7	N	N	Y	Y	7	11
8	Y	Y	N	N	106	66
9	N	Y	N	N	106	75
10	Y	N	Y	N	159	101
11	N	N	Y	N	58	89
12	Y	N	N	Y	230	208
13	N	N	N	Y	164	146

Table 5.2: A full categorisation of the results for the 1721 problems in the test set. A Y indicates that a heuristic selected an optimal variable ordering, or that machine learning selected an optimal heuristic; a N indicates that a heuristic did not select an optimal variable ordering, or that machine learning did not select an optimal heuristic.

There are some interesting features of Table 5.2. For a significant proportion of examples (23.2% for quantifier-free and 33.3% for quantified examples) all three heuristics select an optimal ordering (not necessarily the same ordering, or indeed the best ordering). In the case of two heuristics selecting an optimal ordering, the most common case is when `sotd` and Brown select an optimal ordering, but `ndrr` does not. When only one heuristic selects an optimal ordering the most common case is when only Brown selects an optimal ordering.

We can analyse the results to compare the behaviour of the heuristics for all 7001 examples. The complete results for the heuristics are analysed further in Section 5.3.5.

The important comparison in Table 5.2 is between the pairs of rows where machine learning successfully selects an optimal heuristic and does not. We can see that in all cases but one the machine learning algorithm selects an optimal heuristic more often than not (in Cases 8 and 9 machine learning selects optimally for 50% of Quantifier-Free examples and 47% of quantified examples).

These comparisons show clearly the benefit of using machine learning: for example, considering cases 4 and 5 we see that machine learning selects an optimal ordering 86% and 84% of the time. In these cases two heuristics select optimal orderings, and so if we chose a heuristic randomly, we would have a 67% chance of selecting an optimal

sotd	ndrr	Brown	Quantifier-Free	Quantified	Random Choice
Y	Y	N	79%	80%	67%
Y	N	Y	86%	84%	67%
N	Y	Y	90%	84%	67%
Y	N	N	50%	47%	33%
N	Y	N	73%	53%	33%
N	N	Y	58%	59%	33%

Table 5.3: Proportion of successful choices of an optimal heuristic by machine learning, in comparison to the chance of a random choice selecting an optimal heuristic.

	Machine Learning		sotd		ndrr		Brown	
Quantifier-Free	1312	76.2%	1039	60.4%	872	50.7%	1107	64.3%
Quantified	1333	77.5%	1109	64.4%	951	55.3%	1270	73.8%

Table 5.4: Total number of problems for which machine learning and each heuristic is optimal.

heuristic. For all cases where either one or two heuristics are optimal, we can compare the use of machine learning with a random choice: as shown in Table 5.3. We can see that machine learning does significantly better than random choice in all cases, often by a startling degree.

Obviously, given a new problem there is no way of immediately knowing which of the heuristics will be optimal (otherwise we would simply select the optimal heuristic) and so whilst Tables 5.2 and 5.3 are useful for analysing the performance of machine learning on the test examples, they are not helpful in predicting performance on a new problem. Table 5.4 gives the total number of problems (out of 1721) for which each heuristic and machine learning is optimal.

Considering the heuristics alone it seems that Brown is the heuristic that is most often optimal (with `sotd` competitive), whilst `ndrr` performs relatively poorly. This will be discussed further in Section 5.3.5 where the data for all 7001 examples will be considered.

It is clear from Table 5.4 that using machine learning is better than using a single heuristic. To compare the overall behaviour of machine learning and selecting a heuristic at random we need to summarise the data in Table 5.2 according to the number of heuristics that are optimal in each case. For quantifier-free problems there are 399 where all heuristics are optimal (Case 1), 499 where two are optimal (Cases 2-7), and 823 where only one is optimal (Cases 8-13). Therefore the expected proportion of optimal heuristics

if chosen at random is 58.5%. In the quantified case there are 573 where all heuristics are optimal (Case 1), 463 where two are optimal (Cases 2-7), and 685 where only one is optimal (Cases 8-13). Therefore the expected proportion of optimal heuristics if chosen at random is 64.5%.

We can therefore say that machine learning performs significantly better than any individual heuristic or using a random heuristic. It offers an increase in performance compared to random choice and the best performing heuristic (Brown):

- **Quantifier-free:**
  - Random Choice: 58.5%;
  - Brown's Heuristic: 64.3%;
  - Machine Learning: 76.2%.
- **Quantified:**
  - Random Choice: 64.5%;
  - Brown's Heuristic: 73.8%;
  - Machine Learning: 77.5%.

It should be noted that all the results given here were specifically for problems in three variables and fully existentially quantified. There is therefore no guarantee that this SVM would be appropriate for any other class of examples. It would be interesting to conduct a thorough investigation to see how appropriate this application of machine learning is for other classes of CAD problems. Machine learning is therefore superior to the known methods of selecting a variable ordering.

5.3.4 Future work on Machine Learning

There are many ways in which this work could be extended to futher explore the benefit machine learning can offer in the formulation of problems for CAD, and there are plans to tackle a range of these in further collaboration between the two research groups.

Extending current investigation

Whilst a large corpus of data was used in this investigation, the data set was rather uniform (three variables, existential quantifiers, same source). An obvious extension to the work in this section is to apply machine learning to a wider set of examples to verify its efficacy (along with the superiority of Brown's heuristic). This could be investigated first by altering the quantifiers of the current set of examples (although if not uniformly existential or universal this would limit the permissible variable orderings), or considering examples from the NLSAT database with different numbers of variables.

There is also the option to use an expanded set of heuristics in the experimentation. There are variants on `sotd` and `ndrr` (applied greedily or on different input sets) as well

as hybrid heuristics. Adding more heuristics may, however, decrease the accuracy of the SVM.

We have also singularly used QEPCAD for all CAD construction. Other implementations could be considered, and an attempt made for machine learning to select an optimal choice.

There are also many questions relating to the machine learning choices for this experiment that could be explored. The use of SVM as the machine learning method is not the only choice and other machine learning techniques could be investigated with the same data set to compare performance. Further, the choice of feature vector for the SVM is not predetermined and can be investigated further.

Applying Machine Learning to Gröbner Preconditioning

In Chapter 6, Gröbner preconditioning is investigated. This generally proves beneficial and reduces the cell count of the resulting CAD, but this effect is not universal. To help identify when preconditioning is useful, a metric `TNoI` is introduced (Definition 6.7), which proves highly effective (but not universally so) at predicting when the preconditioning should be applied.

In Section 6.2.9 it is suggested that machine learning could be useful to help predict the benefit (or detriment) of preconditioning. This is obviously an important question for computer algebra, but such an investigation could also offer an insight to the machine learning. Machine learning could be applied in the two following ways:

- **Indirectly:** Use machine learning to pick the most appropriate heuristic for deciding whether to precondition.
- **Directly:** Use machine learning directly to decide whether preconditioning should be used for a given problem.

It would be insightful to compare the performance of both these approaches.

5.3.5 Further Analysis of the Heuristic Data

In the process of applying machine learning to pick a heuristic for selecting a variable ordering, a large amount of data was generated. For each of the 7001 three-variable examples in the NLSAT database a CAD was constructed for all six variable orderings, and all three heuristics were used to predict a variable ordering. Previous work on CAD heuristics has involved small data sets ([DSS04] used 48 examples to obtain their conclusions), so such a large data set allows for fresh insight. This was considered

	sotd		ndrr		Brown	
Quantifier-Free	4221	60.3%	3620	51.7%	4523	64.6%
Quantified	4603	65.8%	4000	57.1%	5166	73.8%

Table 5.5: Total number of problems for which each heuristic is optimal from the 7,001 three-variable problems in NLSAT database.

	Mean			Median		
	sotd	ndrr	Brown	sotd	ndrr	Brown
Quantifier-Free	27.3%	−0.2%	25.3%	29.5%	0.0%	32.3%
Quantified	19.5%	4.2%	21.0%	14.7%	0.0%	16.7%

Table 5.6: Savings for each heuristic compared to the average cell count over all six variable orderings. The results were computed with the 5,262 quantifier-free and 5,332 quantified problems for which no variable ordering timed out.

by members of the research groups at Bath and Cambridge and published as a poster abstract [HEW+14a]. The author was involved in discussions of the results but did not conduct the analysis.

For each of the 7001 examples (in both quantifier-free and fully existentially quantified formats) we can record whether each heuristic selects an optimal variable ordering. Table 5.5 shows these values for each heuristic. We can see that, for both quantifier-free and quantified problems, the Brown heuristic selects an optimal variable ordering most often. This highlights the strength of the heuristic, especially when coupled with the fact that it is computationally cheap and simple to implement.

We can also see from Table 5.5 that `sotd` is a competitive heuristic, but `ndrr` performs worse than the other choices. This is perhaps indicative of the fact that `ndrr` was initially created to handle cases that `sotd` fails to identify, and designed as a heuristic to break ties.

Whilst selecting an optimal variable ordering is important, it is also relevant to consider the actual savings in cell counts. When a heuristic selects a non-optimal variable ordering it may differ from the optimal choice by as little as 2 cells or as many as thousands of cells. Table 5.6 summarises this behaviour by computing the average cell count for each problem over the six variable orderings, then computing the percentage saving (with a negative percentage indicating an increase in cell count) for the variable ordering each heuristic selects. The mean and median of the savings of each heuristic are given in Table 5.6.

The data used to construct Table 5.6 is also summarised in Figure 5.1. This figure

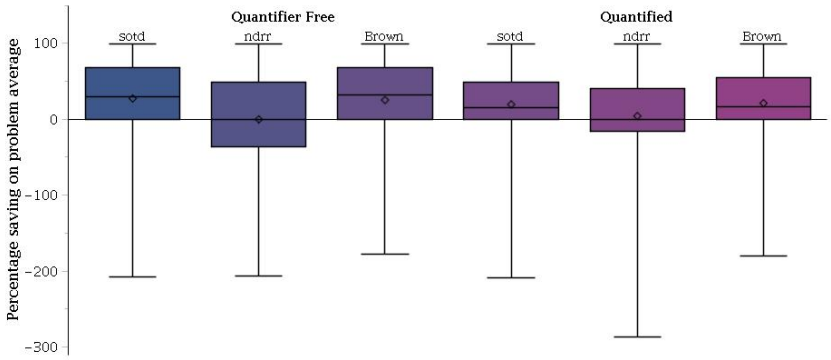


Figure 5.1: Box plot for the percentage saving in cell counts for each heuristic. The range of the data is indicated (discounting outlier values), interquartile range, mean, and median.

	`sotd`		`ndrr`		Brown	
Quantifier-Free	559	32.1%	537	30.9%	594	34.2%
Quantified	512	30.7%	530	31.8%	478	28.6%

Table 5.7: Total number of problems for which each heuristic avoids a time out. The results are with respect to the 1,739 quantifier-free and 1,669 quantified problems for which at least one variable timed out.

displays the means and median of each data, along with the interquartile range of the data and overall range. It discounts any outliers, which are points further than $\frac{3}{2}$ times the interquartile range away from the upper and lower quartiles.

In most cases the performance of the heuristics is similar, and resembles their optimality: Brown offers the greatest savings, with `sotd` offering a slightly smaller saving, and `ndrr` performing relatively poorly (and in one case proving worse than average). For quantifier-free examples `sotd` offers a slightly better mean saving, although has a lower median than Brown.

The saving in cell count is not necessarily the most important metric, and there are cases where it may be more important to simply ensure that the CAD construction finishes. Of the 7001 examples, 1739 quantifier-free and 1669 quantified problems timed out for at least one variable ordering. Table 5.7 gives the number of these examples where each heuristic avoids a time out. Table 5.7 shows that for quantifier-free problems the Brown heuristic is also the best at guaranteeing completion. However, for quantified problems it performs poorly, with `ndrr` being the most effective at selecting a feasible ordering.

To summarise the work on existing heuristics it is evident that Brown is clearly the best choice in general. Not only is it the cheapest to compute (requiring no projection or further computation) but it picks an optimal ordering more often than `sotd` and `ndrr`. It offers good savings over the average cell count (along with `sotd`) and is the most effective at choosing feasible orderings for quantifier-free problems (although it performs the worst out of the heuristics for quantified problems).

The data used for these conclusions, as with the machine learning experiment, is of a particular format: three variables with all quantifiers being existential. It is therefore important to consider these results within that context, and there is no guarantee that similar results will be achieved on a different or more varied data set (and this would be interesting future work). However, it is compelling evidence and the largest investigation into CAD heuristics that the author knows of.

5.3.6 Machine Learning Conclusions

It is clear from the work throughout this section that machine learning can be used to great effect within computer algebra. Applying machine learning (using support vector machines) to the task of selecting a variable ordering for CAD it is necessary to approach the problem indirectly, by selecting a heuristic to then choose a variable ordering.

Machine learning selected an optimal heuristic for 76.2% of quantifier-free problems and 77.5% of quantified problems. This is better than the best-performing heuristic of Brown (by 11.9% and 3.7%, respectively) and also better than selecting a heuristic at random (by 6.0% and 1.3%, respectively). Machine learning also proves to be beneficial in nearly all individual cases relating to which heuristics are optimal.

Using the results of all $7,001$ examples from the NLSAT database that were used for the experimentation, it was also shown that Brown's heuristic outperforms `sotd` and `ndrr`. Combined with the very small computation cost, it is clear that if machine learning is not available then Brown's heuristic is a great alternative, with `sotd` performing only slightly worse. It also highlighted that `ndrr` as an individual heuristic performs rather poorly (and is very costly), and so it is best suited to be used within a hybrid heuristic to break ties.

5.4 CAD Dimensional Distribution

In Section 4.3 the idea of a layered sub-CAD was introduced, consisting of all cells with a specified dimension or greater. This motivates the investigation of the distribution of

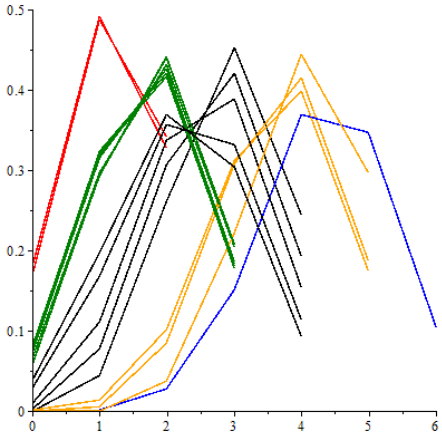


Figure 5.2: Dimensional distributions for a selection of examples from [CMXY09] and [BH91] separated according to the number of variables.

dimensions of cells within a given CAD. This seemingly innocuous question proves both interesting and inspires a new heuristic for variable ordering described in Section 5.4.4. This work was submitted for publication in [WEBD14] and is based on work in [WE13].

We introduce some notation for the size of each layer of cells in a CAD or sub-CAD:

Definition 5.8.
Let $\mathcal{D}$ be a CAD or sub-CAD of $\mathbb{R}^n$. Let $\mathfrak{D}_l$ be the number of cells of $\mathcal{D}$ of dimension l, for $l = 0, \ldots, n$. For a CAD $\mathcal{D}$ of $\mathbb{R}^n$ we define the **dimensional distribution** to be the list

$$[\mathfrak{D}_0, \mathfrak{D}_1, \ldots, \mathfrak{D}_n].$$

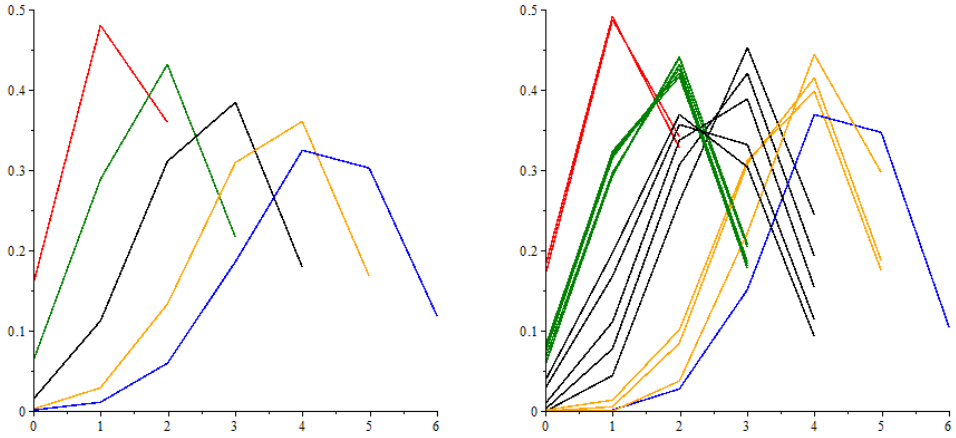
5.4.1 Empirical Investigation

We consider a variety of empirical evidence regarding the dimensional distribution of CADs.

CAD Repository Data

Initially, two collections of examples from [WBD13] (those sourced from [CMXY09] and [BH91]) were inspected. The dimensional distributions were plotted and showed a startling regularity for problems with the same number of variables.

Figure 5.2 shows the dimensional distribution for the examples in [CMXY09] and [BH91] respectively. The distributions are separated, by colour, according to the number of variables (ranging from two to six variables).



(a) Binomial distributions $(n, p) = [(2, 0.6), (3, 0.6), (4, 0.65), (5, 0.7), (6, 0.7)]$.

(b) Dimensional distributions for [CMXY09, BH91].

Figure 5.3: Binomial distributions and dimensional distributions of examples from [CMXY09] and [BH91].

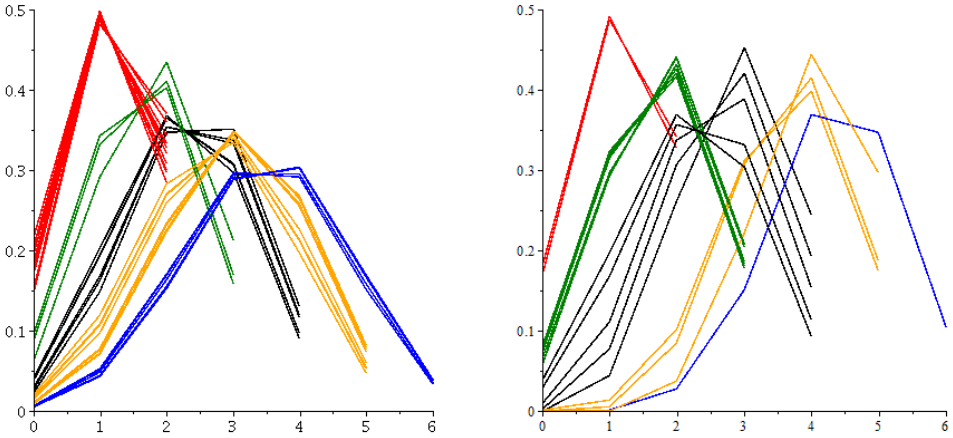
Binomial Distributions

All the graphs in Figure 5.2 exhibit a clear shape similar to a normal distribution that is biased towards cells with large dimension. An emulation of this can be created with the binomial distribution.

Recall that the **binomial distribution** for n trials with probability p of success is given by:

$$\mathbb{P}(X = x) := \begin{cases} \binom{n}{x} p^x (1-p)^{n-x} & 0 \leq x \leq n \\ 0 & \text{otherwise} \end{cases}.$$

We can consider a binomial distribution with a value of p greater than 0.5 to give a bias similar to what was exhibited in the dimensional distributions of Figure 5.2. In Figure 5.3a a binomial distribution is shown for n ranging from 2 to 6. with p values selected by eye, increasing from 0.6 to 0.7. These distributions are shown alongside Figure 5.3b which shows the corresponding dimensional distributions from [CMXY09] and [BH91]. It would seem that as n increases, then the appropriate value of p also increases, which suggests a greater shift towards higher dimensional cells, however there is also less data to compare for large n so this may not be a general trend.



(a) Combinatorially random CADs.

(b) The [CMXY09] and [BH91] examples.

Figure 5.4: The dimensional distributions of 45 combinatorially random CADs (with variables $2 \leq n \leq 6$ and number of sections $1 \leq s \leq 7$) with the dimensional distributions from examples in [CMXY09] and [BH91]

Combinatorially Random CADs

It would seem from the regularity of Figure 5.2 that the distribution of cells is relatively unaffected by the specific polynomials used to generate the CAD. To test this idea, we consider **combinatorially random CADs**: these are constructed by selecting a random number of variables, and splitting each cylinder over a cell into a random number of cells. The construction is done in MAPLE using its `rand` command to construct lists of cell indices representing the theoretical cells. This is much quicker than constructing CADs for random polynomials and is obviously unrelated to a choice of polynomials and intentionally independent of any underlying real algebraic geometry.

Figure 5.4a shows the dimensional distribution of 45 random combinatorially random CADs. Each CAD had a random number of variables chosen from $\{2, \ldots, 6\}$ and each cylinder was split according to a random number of sections chosen from $\{1, \ldots, 7\}$ (therefore having 3 to 15 cells). This is given alongside the examples from [CMXY09] and [BH91] in Figure 5.4b and it is clear that they have a similar distribution, although there are obviously some differences.

It is worth noting that for both examples and random constructions the top two layers often form a large proportion of the cells. This is unfortunate, as 2-layered sub-CADs can be useful for applications such as adjacency (discussed further in Appendix A).

5.4.2 Combinatorial Investigation

As Figures 5.3 and 5.4 suggest the dimension distribution is independent of the real algebraic geometry, we now consider the underlying combinatorial structure of a CAD. To do this we strip away the reliance on input polynomials and consider the combinatorial construction of a CAD in the following manner.

Lemma 5.2.
Let $\mathcal{D}$ be a partition of $\mathbb{R}^n$ constructed by the following:

1. *Decompose $\mathbb{R}^1$ using k_1 0-cells.*
2. *When lifting from the $\mathbb{R}^m$ to $\mathbb{R}^{m+1}$ decompose the cylinder over a cell of dimension m' using k_m (m')-cells.*

Decomposing $\mathbb{R}^n$ this way gives:

$$\mathfrak{D}_l = \sum_{\substack{L\subseteq[n]\\|L|=l}} \left(\prod_{i\in L}(k_i+1) \prod_{j\in[n]\setminus L} k_j \right),$$

where $[n]$ is the combinatorial notation for $\{1,\ldots,n\}$.

In particular we have:

$$\mathfrak{D}_0 = \prod_{i=1}^{n} k_i, \quad \mathfrak{D}_n = \prod_{i=1}^{n}(k_i+1).$$

Proof.
The dimension of a cell in $\mathcal{D}$ is equal to the sum of the parity of its cell indices. For a cell to have dimension l, it must therefore have l odd indices and $n-l$ even indices.

We can characterise an l-dimensional cell by the position of its odd indices. Call the set of these positions L. For a fixed L there are many cells associated to it. For level 1, there are a total k_1+1 choices of 1-cells if $1 \in L$ and k_1 choices of 0-cells if $1 \notin L$. Continuing to build the CAD, at level i there are k_i+1 cell choices if $i \in L$ and k_i choices if $i \notin L$.

Therefore, for a fixed L, the number of cells that have an appropriate cell index is given by:

$$\prod_{i\in L}(k_i+1) \prod_{i\in[n]\setminus L} k_i.$$

All that remains is to sum over all possible subsets L of $[n]$ with cardinality l.

□

This is a major simplification of the problem at hand, however it does well to model standard CAD behaviour empirically.

It is very easy to see that if $k_i = k$ for all i then the sequence $\{\mathfrak{D}_l\}$ is simply the sequence of binomial coefficients of $(k + (k + 1)x)^n$. This is proven in the following lemma.

Lemma 5.3.
Let $\mathcal{D}$ be as given in Lemma 5.2. Then the generating function for $\mathfrak{D}_l$ is given by:

$$\Gamma(x) := \prod_{i=1}^{n}(k_i + (k_i + 1)x).$$

That is, $\mathfrak{D}_l$ is the coefficient of x^l in the expansion of $\Gamma(x)$.

Proof.
Expanding out $\Gamma(x)$, x^l is obtained precisely by choosing x from l different linear factors. This amounts to selecting l integers from the set $[n]$. For a given L, each $i \in L$ contributes $k_i + 1$ to the coefficient of the generated monomial, and each $i \notin L$ contributes k_i. This means the coefficient of the generated x^l is:

$$\prod_{i\in L}(k_i + 1) \prod_{i\in[n]\setminus L} k_i.$$

The coefficient of x^l in $\Gamma(x)$ is precisely the summation of all such coefficients:

$$\sum_{\substack{L\subseteq[n]\\|L|=l}} \left(\prod_{i\in L}(k_i + 1) \prod_{j\in[n]\setminus L} k_j \right),$$

which was shown in Lemma 5.2 to be $\mathfrak{D}_l$.

□

Lemma 5.3 certainly lends some credibility to the idea that the dimension of cells in a CAD roughly obeys a binomial statistical distribution.

It may seem at first like this construction has somehow avoided the doubly-exponential complexity of CAD. This is not the case: taking a resultant at each level in projection results in an increase of each degree by a factor of 2^n.

Variables	2	3	4	5
Fraction	0.334	0.192	0.161	0.181

Table 5.8: Average fraction of full-dimensional cells for examples sourced from [WBD13].

5.4.3 Estimation of CAD size

This consistency in dimensional distribution can be of great use. As a one-layered CAD is generally easy to compute we can use it to predict the size of a complete CAD.

The obvious way to do this is to compute the dimensional distribution for a collection of examples with the same number of variables and take the average of the fraction of full cells in each. Multiplying the number of cells for the 1-layered CAD in question by the reciprocal of this average should give a reasonable estimate for a complete CAD.

Computing values for examples sourced from [WBD13] we can also calculate average fractions of full cells in distributions for a given number of variables. These results are shown in Table 5.8.

Remark 5.4.
We can also create random distribution fractions by using the formulae obtained in Lemma 5.2 so that:

$$\frac{\mathfrak{D}_l}{\sum_{i=1}^{n}\mathfrak{D}_i} = \frac{\sum_{\substack{L\subseteq[n]\\|L|=l}}\left(\prod_{i\in L}(k_i+1)\prod_{j\in[n]\setminus L}k_j\right)}{\prod_{i=1}^{n}(2k_i+1)}$$

and in particular the fraction the top layer constitutes is given by the simple formula:

$$\frac{\mathfrak{D}_n}{\sum_{i=1}^{n}\mathfrak{D}_i} = \frac{\prod_{i=1}^{n}(k_i+1)}{\prod_{i=1}^{n}(2k_i+1)}.$$

This simplifies even further when all the k_i are equal, simply giving:

$$\frac{\mathfrak{D}_n}{\sum_{i=1}^{n}\mathfrak{D}_i} = \left(\frac{k+1}{2k+1}\right)^n.$$

Obviously using an averaged value to predict the size of a complete CAD will not work universally but initial results are promising, as shown in the following example.

Example 5.1.
Two random polynomials in x, y, z were created, each with total degree 2:

$$g := 81zy - 3zx - 88yx + 99x^2 - 12y - 48; \tag{5.1}$$

$$h := 80z^2 + 40zy - 41y^2 + 44yx - 28z + 11. \tag{5.2}$$

These were input into the CAD algorithms under the two variable orderings: $x \prec y \prec z$ and $x \succ y \succ z$.

With variable ordering $x \prec y \prec z$ a 1-layered CAD was produced with 372 cells, which gives a predicted complete CAD of 1941 cells. In reality, a complete CAD produced by McCallum's projection contains 2057 cells, which is a difference of 116 (around 5%).

With variable ordering $x \succ y \succ z$ a 1-layered CAD was produced with 454 cells, which gives a predicted complete CAD of 2368 cells. In reality, a complete CAD produced by McCallum's projection contains 2373 cells, which is a difference of only 5 cells (around 0.2%).

From experimentation, it would seem that larger CADs have more accurate predictions, which is to be expected. For example when dealing with only a single polynomial with a CAD of at most 200 cells the results can be inaccurate but with more polynomials and CADs over 1000 cells the predictions seem to mostly be within 5%. Arguably, the larger examples are those for which an accurate prediction is most important.

Indeed, it seems the most appropriate use of this approximation is estimating feasibility of problems and predicting good variable orderings. This will be discussed in Section 5.4.4.

5.4.4 Cell Dimension Heuristic

We can use the ideas behind the dimension distribution of cells in a CAD as a method of selecting a variable ordering.

We consider a motivating example before describing the general heuristics.

Example 5.2.
We consider the set of random polynomials in three variables:

$$F := \left\{x^2 + y - z^3 - 1, x^2 - 5y + 1, z^3 - xy, z^3 - 5\right\}.$$

We wish to know which of the six possible variable orderings gives the smallest CAD. We proceed by computing the six possible 1-layered sub-CADs.

Order	Cells			Time	
	1-LCAD	Prediction	Complete CAD	1-LCAD	Complete CAD
$z \prec y \prec x$	544	2833	2949	1.112	11.734
$y \prec z \prec x$	710	3698	3995	1.025	13.870
$z \prec x \prec y$	**264**	**1375**	**1299**	0.758	**5.033**
$x \prec z \prec y$	312	1625	1545	**0.527**	5.784
$y \prec x \prec z$	592	3083	3207	0.971	12.955
$x \prec y \prec z$	448	2333	2347	0.711	9.006

Table 5.9: Use of 1-layered sub-CADs as a heuristic for F. Cell counts and timings are given for 1-layered sub-CADs and complete CADs. The predicted cell count is also given: obtained by multiplying the 1-layered sub-CAD cell count by 1/0.192.

The results for F are given in Table 5.9. We see that the 1-layered sub-CAD cell counts predict that $z \prec x \prec y$ gives the smallest complete CAD, which is indeed correct (the ranking of the variable orderings is equal for the 1-layered and complete CADs). It is worth noting that the timings are less clear, with $z \prec x \prec y$ being the third quickest to produce a 1-layered CAD, but the quickest to produce a full CAD. This highlights how cell count is a more useful and consistent measure for CAD complexity. The total time to compute all 1-layered sub-CADs for F is 5.104 seconds which means that it takes, in total, 10.137 seconds to predict and construct the complete CAD for $z \prec x \prec y$. Constructing the complete CAD for $y \prec z \prec x$ directly takes 13.870 seconds and so this heuristic offers a practical saving of 3.733 seconds from the worst case (and a saving of 2696 cells). With respect to the average of all six variables the 1-layered heuristic incurs a slight cost of 0.410 seconds (but saves 1258 cells).

We formally define the layered heuristic.

Definition 5.9.
Given a set of input polynomials and set of permitted variable orderings, the **layered heuristic** computes the 1-layered sub-CAD with respect to each of the given variable orderings and selects the one producing the smallest sub-CAD.

The layered heuristic (for a complete set of variable orderings) is described in Algorithm 5.1. The one layered sub-CADs for each variable ordering can be constructed using either the direct or recursive sub-CAD algorithms (described in Algorithms 4.3 and 4.4), with the latter offering the benefit of not repeating computations.

Obviously this may not necessarily be a practical heuristic. For small examples (as shown for F in Example 5.2) the time computing $n!$ 1-layered sub-CADs may be more costly than the average time saved by picking the near-optimal variable ordering for the

Algorithm 5.1: `LayeredHeuristic(F, vars)`: Basic layered heuristic algorithm.

Input : A set of polynomials F, a set of variables $vars$.
Output: The predicted optimal variable ordering $optvars$, and a CAD, $\mathcal{D}$, for F with respect to $optvars$.

```
1 V ← combinat[permute](vars);                    // All variable orderings
2 mincells ← ∞;
3 for v ∈ V do
4 |   L_v ← LCAD(F, 1, v);                          // 1-layered sub-CAD
5 |   if |L_v| < mincells then
6 |   |   optvars ← v;                  // If smallest, set to optvars
7 D ← FullCAD(F, optvars, [L_optvars]);           // Construct complete CAD
8 return [optvars, D];
```

complete CAD. For large examples (especially in many variables) the computation time for the $n!$ 1-layered sub-CADs may simply be too large. This is investigated in Section 5.4.5.

Computing a collection of 1-layered CADs is certainly feasible as a tie-breaking heuristic. We know that all the heuristics mentioned in this chapter can have trouble distinguishing between variable orderings (i.e. coupled variables with Brown's heuristic) and so the size of the 1-layered CADs for the set of potential variable orders can be used as a tie-breaker. It may also be the case that, due to restrictions on variable ordering due to quantifiers, there are only a small number of possible variable orderings to check.

Parallel Implementation

We can improve the efficiency of the layered heuristic by computing the 1-layered sub-CADs in parallel. We describe two potential algorithms, neither of which has yet been implemented. With the MAPLE `Threads` package, these could be interfaced with the `ProjectionCAD` module.

Algorithm 5.2 describes a basic parallel algorithm for the layered heuristic across a set of cores. Each 1-layered sub-CAD algorithm is computed in parallel across the threads. As soon as one sub-CAD finishes computation all other computations are terminated (this may not be the optimal ordering choice but it will be near-optimal). The remaining lifting calls are then computed in parallel.

Algorithm 5.3 is slightly more sophisticated and also guarantees that the variable ordering with the smallest 1-layered sub-CAD is selected. The sub-CAD algorithms are again launched in parallel, but now any time a sub-CAD finishes construction its size is

Algorithm 5.2: `ParallelLayeredHeuristic(F, vars)`: Parallel layered heuristic algorithm (basic).

Input : A set of polynomials F, a set of variables $vars$.
Output: The predicted optimal variable ordering $optvars$, and a CAD, $\mathcal{D}$, for F with respect to $optvars$.

```
1  V ← combinat[permute](vars);                          // All variable orderings
2  for v ∈ V do in parallel
3      launch L_v, Uneval_v ← LCADRecursive(F, v);       // 1-layered sub-CAD
4  optvars ← first v for L_v to finish;
5  foreach v ∈ V \ {optvars} do
6      abort L_v;                                        // Cancel other sub-CADs
7  repeat
8      for c ∈ Uneval_optvars do in parallel
9          l_c, uneval_c ← GenerateStack(F, c);          // Parallel lifting
10         L_optvars ← L_optvars ∪ l_c;
11         Uneval_optvars ← Uneval_optvars ∪ Uneval_c;
12 until Uneval_optvars is empty;
13 return [optvars, L_optvars];
```

compared to the current optimal choice and the larger is aborted. Note that the parallel lifting of Algorithm 5.2 can also be used, although more care would be needed in thread management.

5.4.5 Experimental Investigation of 1-Layered Heuristic

We now proceed with a more thorough investigation of the layered heuristic (using Algorithm 5.1). We consider a collection of 75 random examples of the form: $[f_1, f_2, f_3]$ where f_1 and f_2 are random quadratic polynomials and f_3 is a random linear polynomial in variables $\{x, y, z\}$ (the f_i were generated with Maple's `randpoly` command).

It is obvious that the 1-layered heuristic is well suited for the use of the recursive layered CAD algorithm described in Algorithm 4.4 and implemented in `ProjectionCAD`. We therefore consider first computing the six 1-layered sub-CADs using `LCADRecursive` followed by computing the complete CAD recursively for the predicted variable ordering (choosing the first lexicographically with respect to $x \prec y \prec z$ if there are multiple choices). Being able to compute the complete CAD using `LCADRecursive` prevents the recomputation of the 1-layered sub-CAD and so offers an overall saving to separate computation of the 1-layered sub-CADs and complete CAD.

Algorithm 5.3: `ParallelLayeredHeuristic(F, vars)`: Extended parallel layered heuristic algorithm.

Input : A set of polynomials F, a set of variables $vars$.
Output: The predicted optimal variable ordering $optvars$, and a CAD, $\mathcal{D}$, for F with respect to $optvars$.

```
1  V ← combinat[permute](vars);                    // All variable orderings
2  mincells ← ∞;
3  for v ∈ V do in parallel
4  |  B_v ← false;
5  |  launch L_v ← LCAD(F, 1, v);                  // 1-layered sub-CADs
6  |  if complete B_v ← true;
7  |  launch D_v ← FullCAD(F, v, [L_v]);           // Complete CAD
8  |  if complete optvars ← v;          // Set first to complete to optvars
9  foreach v ∈ V such that B_v = true do
10 |  for w ∈ V such that w ≠ v and B_w = true do
11 |  |  if |L_w| < |L_v| then
12 |  |  |  abort D_v;                            // Abort larger ordering
13 |  |  else
14 |  |  |  abort D_w;                            // Abort larger ordering
15 when optvars is assigned: return [optvars, L_optvars];
```

Tables 5.10a and 5.10b show the performance of the layered (recursive) heuristic on the 75 random examples. The results from Tables 5.10a and 5.10b are summarised in Figures 5.5a and 5.5b.

It can immediately be seen that the layered heuristic always offers a saving in cell count, and often this is substantial compared to both the average and worst variable orderings. The results are less clear for timings, with most examples showing an overall saving in time (sometimes quite substantial) but with a portion being slower than the average, or even the worst, case. The risk of taking a little longer to compute the CAD must be weighed up against the savings in cells.

Although it can sometimes take longer to use the 1-layered heuristic than to compute a CAD directly, it has the distinct benefit of being hugely effective at providing a small CAD as output. If the CAD is to be used in a further application then the 1-layered heuristic is a very good way to pick a variable ordering.

Remark 5.5.
If the CADs we are constructing are strong cell decompositions (Definition A.3 related to adjacency) then it seems clear that the full-dimensional cells are perfectly correlated with

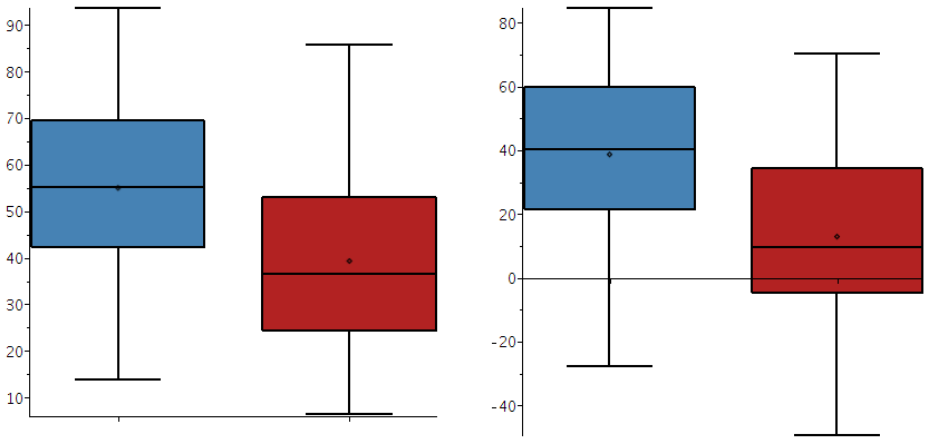
Cells	vs Maximum	vs Average
Mean	4719 55.0%	2220 38.7%
Best	12816 93.6%	5204 84.6%
Worst	762 13.9%	297 6.49%

(a) Comparison of cell counts.

Time	vs Maximum	vs Average
Mean	64.3 38.7%	10.0 12.9%
Best	631.9 84.6%	143.3 70.1%
Worst	−44.1 −27.9%	−66.1 −49.3%

(b) Comparison of timings (in seconds).

Table 5.10: Tables demonstrating the use of the layered (recursive) heuristic on 75 random examples in three variables. All examples are of the form $[f_1, f_2, f_3]$ where f_1 and f_2 are random quadratic polynomials, and f_3 is a random linear polynomial (all generated using `randpoly` in MAPLE).



(a) Percentage savings in cell count.

(b) Percentage savings in time.

Figure 5.5: Box plots illustrating the savings of using the 1-layered sub-CAD heuristic. The blue (left) plot indicates the percentage saving compared to the worst variable ordering, and the red (right) plot indicates the percentage saving compared to the average over all six variable orderings.

Technique	Cells	Time	`sotd`	`td`	`ndrr`	1-Lay	Section	Page
PL-CAD (Col)	54037	255.304	67	39	14	5012	2.3	30
PL-CAD (McC)	54037	266.334	67	39	14	5012	2.3	30
EC-CAD (f_3)	20593	65.856	67	39	14	1372	2.4.4	40
EC-CAD (f_4)	22109	102.781	67	39	14	1522	2.4.4	40

Table 5.11: The Solotareff-3 problem with formulation concepts — variable order $a \prec b \prec v \prec u$.

the size of the complete CAD. The full dimensional cells in a strong cell decomposition implicitly define the $(n-1)$-dimensional cells, which inductively define the $(n-2)$-dimensional cells and so forth. Therefore for strong cell decompositions the layered heuristic is completely accurate. This accuracy is not guaranteed if we do not have a strong cell decomposition, although it should be closely correlated, and this should be investigated.

The layered heuristic need not be limited to just variable ordering. It can clearly can be used for other formulation choices such as equational constraints. It can also be made more efficient by constructing a 1-layered variety sub-CAD for the heuristic: this will be an accurate heuristic for variety sub-CADs but not necessarily a complete CAD. The layered heuristic can also be used to help decide the optimal mathematical expression of a CAD, an issue that will be discussed in Chapter 6.

5.5 Solotareff-3

We consider again the Solotareff-3 problem given in 2.12.

$$(\exists\, u)(\exists v)\Big[[3v^2-2v-a=0] \;\wedge\; [v^3-v^2-av-2b+a-2=0]$$
$$\wedge\; [3u^2-2u-a=0] \;\wedge\; [u^3-u^2-au-a+2=0] \;\wedge\; [1\le 4a] \;\wedge\; [4a\le 7]$$
$$\wedge\; [-3\le 4b] \;\wedge\; [4b\le 3] \;\wedge\; [-1\le v] \;\wedge\; [v\le 0] \;\wedge\; [0\le u] \;\wedge\; [u\le 1]\Big]. \quad (5.3)$$

We consider the formulation issues of choosing between the two variable orderings[6], $a \prec b \prec v \prec u$ and $b \prec a \prec v \prec u$, and designating an equational constraint. The relevant data is shown in Tables 5.11 and 5.12

[6]There are two further permissible orderings by swapping u and v, due to the quantifier block structure, but we do not consider them here to prevent excessive calculations.

Technique	Cells	Time	`sotd`	`td`	`ndrr`	1-Lay	Section	Page
PL-CAD (Col)	161317	916.105	76	52	26	14268	2.3	30
PL-CAD (McC)	154527	857.357	75	51	25	13716	2.3	30
EC-CAD (f_3)	48475	175.139	71	48	23	3040	2.4.4	40
EC-CAD (f_4)	63583	324.663	75	51	25	4132	2.4.4	40

Table 5.12: The Solotareff-3 problem with formulation concepts — variable order $b \prec a \prec v \prec u$.

We will consider the following heuristics and metrics: Brown's heuristic from [Bro04]; `sotd` and `td` from [DSS04]; `ndrr` from [BDEW13]; and the 1-layered sub-CAD heuristic introduced in Section 5.4.

Variable Order

We consider the choice of variable order, and examine the appropriate heuristics for $a \prec b \prec v \prec u$ and $b \prec a \prec v \prec u$:

Brown: Both a and b appear with degree 1, but a appears in two quadratic terms, so b should be eliminated before a.
Selection: $a \prec b \prec v \prec u$.

`sotd` **Heuristic:** The projection set of the first variable ordering gives 67, whilst the second gives 76 or 75 (depending on projection operator).
Selection: $a \prec b \prec v \prec u$.

`td` **Heuristic:** The projection set of the first variable ordering gives 39, whilst the second gives 52 or 51 (depending on projection operator).
Selection: $a \prec b \prec v \prec u$.

`ndrr` **Heuristic:** The projection set of the first variable ordering gives 14, whilst the second gives 26 or 25 (depending on projection operator).
Selection: $a \prec b \prec v \prec u$.

1-Layered Heuristic: The 1-layered sub-CAD of the first variable ordering gives 5012 cells, whilst the second gives 14268 or 13716 (depending on projection operator).
Selection: $a \prec b \prec v \prec u$.

We see that all heuristics correctly select the optimal variable ordering. The first four heuristics all complete in a near-instant time, whilst the 1-layered heuristic takes 24

seconds to construct. Whilst this is much longer than the other heuristics, it is small compared to the time to construct the complete CADs: 266 seconds and 857 seconds, respectively.

Machine learning is not suitable for this problem: all experimentation in Section 5.3 was with respect to three variable examples that were either unquantified or fully existentially quantified, and the feature vector cannot be computed for problems with more variables. Future work on the machine learning application will expand its use to allow it to apply to the Solotareff problem.

Equational Constraint Designation

We now consider the selection of an equational constraint for each variable ordering. We use the equational constraint projection operator for the `sotd`, `td`, and `ndrr` metrics, and construct a 1-layered variety sub-CAD for the final heuristic:

- Variable ordering $a \prec b \prec v \prec u$.:

  `sotd` **Heuristic:** All four equational constraints give 67.
  Selection: No choice.

  `td` **Heuristic:** All four equational constraints give 39.
  Selection: No choice.

  `ndrr` **Heuristic:** All four equational constraints give 14.
  Selection: No choice.

  1**-Layered Variety Heuristic:** f_1 and f_2 return **FAIL**, f_3 gives 1372, f_4 gives 1522.
  Selection: f_3.

- Variable ordering $b \prec a \prec v \prec u$.:

  `sotd` **Heuristic:** f_1 and f_2 give 68, f_3 gives 71, f_4 gives 75.
  Selection: f_1 **and** f_2.

  `td` **Heuristic:** f_1 and f_2 give 45, f_3 gives 48, f_4 gives 51.
  Selection: f_1 **and** f_2.

  `ndrr` **Heuristic:** f_1 and f_2 give 21, f_3 gives 23, f_4 gives 25.
  Selection: f_1 **and** f_2.

  1**-Layered Variety Heuristic:** f_1 and f_2 return **FAIL**, f_3 gives 3040, f_4 gives 4132.
  Selection: f_3.

We see some interesting results. For $a \prec b \prec v \prec u$, none of the projection operator heuristics are able to distinguish between the four equational constraints. However, the 1-layered heuristic not only identifies f_3 as the optimal designation, but also indicates that f_1 and f_2 are unsuitable for designation. As we are constructing a layered variety sub-CAD, and with the equational constraint projection operator, this is quicker than when selecting a variable ordering, taking 8 seconds (compared to 66 and 103 seconds to construct the complete CADs).

For $b \prec a \prec v \prec u$, the projection operator heuristics can separate between the designations, but identifies f_1 and f_2 which are not suitable for designation. Again, the layered variety sub-CAD correctly identifies f_3 and returns **FAIL** for f_1 and f_2. This takes 15 seconds, compared to 175 and 325 seconds to construct the complete CADs.

5.6 Conclusion

In this chapter we considered various formulation choices that need to be made before using a CAD algorithm: the variable ordering to use; which equational constraint to designate; how to decompose a formula for TTICAD; and the order of polynomials to consider for incremental algorithms. All of these can have a large effect on the complexity of the constructed CAD. Two existing heuristics, Brown's heuristic and `sotd`, were investigated and a new metric, `ndrr`, introduced. All heuristics are to a certain degree effective, but can also be fooled by constructed examples. Separate heuristics need to be considered for the recent advances in incremental regular chains algorithms for CADs and TTICADs, and these were briefly discussed.

The application of machine learning to select a heuristic for variable ordering was given, and is thought to be the first application of machine learning to computer algebra formulation. Using a support vector machine to select between {Brown, `sotd`, `ndrr`} proves highly effective: selecting an optimal heuristic for 76.2% of quantifier-free problems and 77.5% quantified problems (compared with 58.5% and 64.5% for a random choice). Further analysis of the data used for the machine learning gave new insight into the heuristics and indicated that Brown is the best performing heuristic. There is much scope for applying machine learning to other questions within CAD and future experiments to decide the application of Gröbner preconditioning from Chapter 6 were detailed.

Through empirical and combinatorial investigation, it was demonstrated that CADs generally have the same distribution of cell dimensions (approximately a binomial distribution for a value of $p > 0.5$). It was described how this can be combined with the

1-layered sub-CAD algorithms of Chapter 4 to predict the size of a complete CAD from its full-dimensional cells. This can be extended to a heuristic for selecting a variable ordering. Although this requires the construction of $n!$ 1-layered sub-CADs it was shown to be an effective heuristic for a collection of random examples in 3 variables: saving on average 38.7% in cell count and 12.9% in total time over the average of all six variable orderings.

All of the formulation choices can interact and influence each other. Therefore the heuristics detailed in this chapter should not be considered independently of each other and this is discussed in Chapter 7.

Chapter 6

Mathematical Description of Problems for CAD

Given a specific problem for which CAD is to be used, there may be many ways to state the problem before applying CAD. This is somewhat different to choosing parameters such as variable ordering or equational constraints, as was discussed in Chapter 5. There is a great amount of freedom in how to express a problem mathematically and there can be much debate as to when reformulation becomes simply solving the problem by alternative methods.

Gröbner basis technology can be applied to a system of polynomial equalities and inequalities to precondition a problem before applying a CAD algorithm. We analyse this preconditioning and show that it can often result in a sharp drop in CAD complexity and construction time. This benefit is not universal and a new metric is identified that can be used to predict the behaviour of the preconditioning.

We also investigate the "Piano Mover's Problem" of navigating a ladder through a right-angled corridor. Previously considered infeasible [Dav86] it has been tackled in the literature [Mar89, Wan96, McC97, YZ06] by making geometric deductions about the problem. We provide a feasible formulation that does not rely on geometric reasoning. Further work is needed to consider the adjacency configuration of the produced CAD and thus construct valid paths when possible. We discuss a collection of general strategies inspired by this problem.

Author's Contribution and Publication

The motivating examples in Section 6.1 resulted from discussion with Bradford and Davenport and communications with Brown [Bro12] for [DBEW12]. All other work in this chapter is the author's.

The work in Section 6.2 was published in [WBD12]. The work in Section 6.3 was first given in the Technical Report [WBDE13] and later published in [WDEB13].

6.1 Motivation for Mathematical Reformulation

6.1.1 Motivation for Gröbner Preconditioning

We consider the **cyclic-4** system of polynomials.

Example 6.1.
Let $a \succ b \succ c \succ d$ and consider the system of equations:

$$\begin{aligned} a + b + c + d &= 0 \\ ab + bc + cd + da &= 0 \\ abc + bcd + cda + dab &= 0 \\ abcd - 1 &= 0. \end{aligned}$$

This proves to be difficult to tackle directly for most CAD technology. Using a projection and lifting based approach or the recursive Regular Chains algorithm both time out after a day's computation. Using the incremental Regular Chains approach completes after around 25 minutes, but produces 187,225 cells.

A Gröbner basis is a structured way to represent an algebraic variety, and we can compute such a basis with respect to the pure lexicographic ordering to get:

$$\begin{aligned} 1 - d^4 - d^2c^2 + c^2d^6 &= 0 \\ -c - d + c^2d^3 + d^2c^3 &= 0 \\ d^4b + d^5 - b - d &= 0 \\ c^2d^4 + bc - bd + cd - 2d^2 &= 0 \\ b^2 + 2bd + d^2 &= 0 \\ a + b + c + d &= 0 \end{aligned}$$

This will have the exact same solution set as the original problem (they describe

the same polynomial ideal), so any CAD of the second systems of polynomials will be sufficient to analyse the solutions to the first system of polynomials.

This proves much more efficient input for all three CAD algorithms. Projection and lifting CAD now produces 1569 cells in 8.3 seconds, recursive regular chains CAD produces 621 cells in 6.1 seconds, and incremental regular chains CAD produces 621 cells in just 1.0 seconds.

A key question is to consider whether such a saving is always gained from taking a Gröbner basis, which motivates further investigation into the interaction between various CAD techniques and Gröbner bases. This will be discussed in Section 6.2.

6.1.2 Motivation for Mathematical Reformulation

Whilst investigating verification [DBEW12] a particular example proved too difficult for computation. In private correspondence with Brown [Bro12] (the maintainer of QEPCAD) he illustrated how expressing a problem correctly for QEPCAD, and hence CAD, can make a big difference in feasibility.

Joukowsky's Transformation

The Joukowsky transformation is a conformal map on the complex plane defined as:

$$f: \begin{array}{rl} \mathbb{C} \to & \mathbb{C} \\ z \mapsto & \frac{1}{2}\left(z + \frac{1}{z}\right) \end{array}.$$

The work in [DBEW12] aimed to show that f is a bijection from $\mathbb{D} = \{z \mid |z| > 1\}$ to $\mathbb{C}^{\ddagger} = \mathbb{C} \setminus [-1, 1]$ automatically. This amounts to showing the following quantified formula is equivalent to **TRUE**:

$$\begin{aligned}(\forall\, a)(\forall\, b)(\forall\, c)(\forall\, d)\Big[\big[[a(c^2+d^2)(a^2+b^2+1) - c(a^2+b^2)(c^2+d^2+1) = 0] \wedge \\ [b(c^2+d^2)(a^2+b^2-1) - d(a^2+b^2)(c^2+d^2-1) = 0] \wedge [bd > 0] \wedge [c^2+d^2-1 > 0]\big] \\ \implies \big[[a = c] \wedge [b = d]\big]\Big]. \quad (6.1)\end{aligned}$$

Trying to use this as direct input for QEPCAD proves too difficult with default initialisation settings. Brown points out that using QEPCAD as a "black box" for either quantifier elimination or CAD construction is unwise and suggests the following steps to manually recast the problem.

Initially, Brown takes the negation of (6.1). This converts the universal quantifiers into existential quantifiers and allows the final conclusion (consisting of a conjunction of equalities) to split the problem into a disjunction of two formulae:

$$\begin{gathered}(\exists\ a)(\exists\ b)(\exists\ c)(\exists\ d)\Big[b^2cd^2+a^2cd^2-ab^2d^2-a^3d^2-ad^2+b^2c^3+a^2c^3-ab^2c^2- \\ a^3c^2-ac^2+b^2c+a^2c=0\wedge b^2d^3+a^2d^3-b^3d^2-a^2bd^2+bd^2+b^2c^2d+ \\ a^2c^2d-b^2d-a^2d-b^3c^2-a^2bc^2+bc^2=0\wedge db>0\wedge d^2+c^2-1>0\wedge c-a\neq 0\Big] \\ \vee \\ (\exists\ a)(\exists\ b)(\exists\ c)(\exists\ d)\Big[b^2cd^2+a^2cd^2-ab^2d^2-a^3d^2-ad^2+b^2c^3+a^2c^3-ab^2c^2- \\ a^3c^2-ac^2+b^2c+a^2c=0\wedge b^2d^3+a^2d^3-b^3d^2-a^2bd^2+bd^2+b^2c^2d+ \\ a^2c^2d-b^2d-a^2d-b^3c^2-a^2bc^2+bc^2=0\wedge db>0\wedge d^2+c^2-1>0\wedge d-b\neq 0\Big]\end{gathered} \tag{6.2}$$

There are multiple points that are notable about this formulation. The first is the ability to split the new formulation into two smaller problems: this only reduces the problem by one polynomial for each half, but recall that the complexity is polynomial in the number of polynomials with an exponent that is exponential in n. Each half of equation (6.2) is preceded by existential quantifiers which is beneficial as it can allow for a simpler calculation: only one sample point needs to be found to determine the statement (in this case, no such points exist and so all cells need to be checked). Finally, both halves of (6.2) are conjunctions involving equations, and so are amenable to the theory of equational constraints (in fact the theory of Gröbner preconditioning from Section 6.2 can also be used).

After splitting this disjunction we can attempt to solve both halves of (6.2). Here Brown uses a slightly counter-intuitive step (due to the implementation of QEPCAD rather than a theoretical issue) of leaving c and d free which allows QEPCAD to utilise the inequality $d^2+c^2>1$.

Following all of these manipulations, QEPCAD can solve each half of (6.2) in around 5–6 seconds. Both halves are shown to be equivalent to **FALSE**, and therefore their disjunction is also **FALSE**. As (6.2) is the negation of (6.1), we obtain that the original statement is proven equivalent to **TRUE**.

We investigate how a change in the mathematical description (such as used here) can be beneficial for CAD in Section 6.3.

6.2 Preconditioning by Gröbner Bases

We now describe an extension to the work of [BH91], investigating the effect of Gröbner preconditioning on CAD construction.

6.2.1 Gröbner Bases

We will provide a brief summary of the basic theory of Gröbner bases, first introduced in [Buc65]. Further details can be found in most computer algebra textbooks (such as [VZGG13]).

Definition 6.1.
A **partial order** $<$ on a set is a transitive and non-reflexive relation. A partial order is a **total order** if for any pair (α, β) of elements of the set either $\alpha = \beta$, $\alpha < \beta$, or $\beta < \alpha$ holds. A total order is a **well-order** if any non-empty subset has a least element.

Definition 6.2.
For a given monomial $m \in \mathbb{k}[\mathbf{x}]$ we identify with m the vector of exponents $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in \mathbb{N}^n$. We also use the notation:

$$m = \mathbf{x}^\alpha = x_1^{\alpha_1} \cdot x_2^{\alpha_2} \cdots x_n^{\alpha_n}.$$

A **monomial order** in $\mathbb{k}[\mathbf{x}]$ is a relation $\prec$ on the exponent vectors such that:

1. $\prec$ is a total order;
2. $\alpha \prec \beta$ implies $\alpha + \gamma \prec \beta + \gamma$ for all $\alpha, \beta, \gamma \in \mathbb{N}^n$ (corresponding to multiplication of monomials);
3. $\prec$ is a well-order.

We give two monomial orderings that we will use (although many others exists and are used in applications).

Definition 6.3.
Define the **lexicographic order** $\prec_{\text{lex}}$ using the following relation:

$$\alpha \prec_{\text{lex}} \beta \quad \Leftrightarrow \text{ the leftmost non-zero entry in } \alpha - \beta \text{ is negative.}$$

Define the **inverted lexicographic order** $\prec_{\text{ilex}}$ to be lexicographic order with the variable order inverted (this is not a standard definition but will be useful). That is:

$$\alpha \prec_{\text{ilex}} \beta \quad \Leftrightarrow \text{ the rightmost non-zero entry in } \alpha - \beta \text{ is negative.}$$

Note that the inverted lexicographic order is not the same as the **reverse lexicographic order**, which places α before β if the rightmost non-zero entry in $\alpha - \beta$ is positive.

Definition 6.4.
Given a polynomial $f \in \Bbbk[\mathbf{x}]$ and a monomial order $\prec$, we write $\mathrm{lt}_\prec(f)$, for the **leading term** of f with respect to $\prec$, and $\mathrm{lm}_\prec(f)$, for the **leading monomial** of f with respect to $\prec$.

The **leading term ideal**, $\langle \mathrm{lt}(F) \rangle$, of a set of polynomials $F \subset \Bbbk[\mathbf{x}]$ with respect to a monomial order $\prec$ is the monomial ideal generated by the leading terms of all polynomials in F:

$$\langle \mathrm{lt}(F) \rangle := \langle \mathrm{lt}_\prec(f) \mid f \in F \rangle.$$

Definition 6.5.
Let $\prec$ be a monomial order and I a polynomial ideal in $\Bbbk[\mathbf{x}]$. A finite set $G \subseteq I$ is a **Gröbner basis** for I with respect to $\prec$ if and only if:

$$\langle \mathrm{lt}(G) \rangle = \langle \mathrm{lt}(I) \rangle.$$

We give an equivalent definition of a **Gröbner basis**. G is a basis of the ideal I that satisfies the following condition:

1. For all $f \in I$, there exists a $g \in G$ such that $\mathrm{lm}_\prec(g) \mid \mathrm{lm}_\prec(f)$.

A **reduced Gröbner basis** also satisfies the additional condition:

2. For all $g, g' \in G$ with $g \neq g$, we have $\mathrm{lm}_\prec(g) \nmid \mathrm{lm}_\prec(g')$

The original algorithm to compute a Gröbner basis was given by Buchberger in his PhD thesis [Buc65]. It consists of computing **S-polynomials**:

$$S(f, g) = \mathrm{lcm}(\mathrm{lm}(f), \mathrm{lm}(g)) \cdot \left(\frac{f}{\mathrm{lt}(f)} - \frac{g}{\mathrm{lt}(g)} \right).$$

It can be shown that a criterion for deciding if a basis is a Gröbner basis is to check that all the S-polynomials (for all pairs of polynomials in the basis) reduce to 0 with respect to the basis. Buchberger's algorithm consists of repeatedly taking reduced S-polynomials and adding any non-zero S-polynomials until all reduce to zero.

6.2.2 Key idea

Consider a (possibly quantified) formula in the first order of the reals, Φ, with quantifier-free part $\varphi(x_1, \ldots, x_n)$. Assume the variable ordering is fixed.

Let us assume that φ (or a subformula of φ) has the form:

$$\varphi : \bigwedge_{i=1}^{s} (f_i = 0) \wedge \bigwedge_{j=1}^{t} (g_j *_j 0), \qquad *_j \in \{<, \leq, >, \geq, =, \neq\}. \tag{6.3}$$

Let $\hat{f}_1, \ldots, \hat{f}_{\hat{s}}$ be a Gröbner basis of the f_i, with respect to some given monomial ordering. Then let $\hat{\varphi}$ be defined as follows:

$$\hat{\varphi} : \bigwedge_{i=1}^{\hat{s}} (\hat{f}_i = 0) \wedge \bigwedge_{j=1}^{t} (g_j *_j 0). \tag{6.4}$$

It is clear from the definition of Gröbner bases that the solutions for $\hat{\varphi}$ are exactly the same as the solutions for φ. Therefore we have an equivalent formula to Φ by replacing φ with $\hat{\varphi}$. For convenience, we will denote this preconditioning by $=_G$.

Once we have computed the $\hat{f}_i$ we can further use Gröbner reduction on the g_i with respect to the $\hat{f}_i$, to produce $\hat{g}_1, \ldots, \hat{g}_t$ which have the same sign behaviour as the g_i when the f_i vanish. Therefore we define $\overline{\varphi}$ as follows:

$$\overline{\varphi} : \bigwedge_{i=1}^{\hat{s}} (\hat{f}_i = 0) \wedge \bigwedge_{j=1}^{t} (\hat{g}_j *_j 0). \tag{6.5}$$

This will have the same solutions as φ, and so we have an equivalent formula to Φ and $\hat{\Phi}$ by replacing φ with $\overline{\varphi}$. We will refer to this further reduction by $\rightarrow_G^*$.

6.2.3 Experimentation and analysis

The idea of combining Gröbner bases and CAD was previously investigated in the Technical Report [BH91]. The authors considered problems of the form (6.3) and use a purely lexicographical Gröbner basis ($=_G$) to produce (6.4). Their motivation were the ideas that a pure lexicographic Gröbner basis is "triangularized", the number of projection polynomials may be reduced if the basis has fewer polynomials, and any polynomials in simply the main variable can be used as constraints.

The authors considered five examples (each with two variable orderings), including the special case of the Solotareff-3 example introduced in Sections 1.3 and 2.12. They

showed that, in general, preconditioning a problem by computing a (purely lexicographic) Gröbner basis can be beneficial, often showing a very substantial speed-up in the total computation time.

Improvements to algorithms (and their implementations) has done much to speed up CAD construction and Gröbner basis computation since [BH91]. However, when recomputing the examples from [BH91] with modern technology the results remain largely the same [WBD12]: preconditioning by computing a lexicographical Gröbner basis generally makes the construction of a CAD for quantifier elimination more efficient. The main difference between the results is that the computation time for the Gröbner bases is largely insignificant in the modern results, whereas there were examples in [BH91] where the cost of computing a basis cancelled out an improvement in CAD construction. All Gröbner bases in this chapter were computed in under 0.03 seconds and therefore only the total computation times (for Gröbner basis and CAD) are given.

The authors of [BH91] note the substantial improvement offered in most cases, but acknowledge that it can be detrimental. They state their plan to research further into the area to try and give an explanation of why the preconditioning works. They finish by stating an aim to "specialise the Gröbner bases algorithm for the use as a preprocessor to quantifier elimination algorithm." Unfortunately, no further research was published by the authors on this topic.

[BH91] with Current Technology

In [BH91] the authors considered using Gröbner preconditioning with an early version of QEPCAD. It seems obvious to investigate their preconditioning tests with other methods of constructing CADs. The same set of examples are considered in Table 6.1.

Table 6.1 compares `CADFull` from `ProjectionCAD` (using McCallum's projection operator) with the recursive approach to building CAD through `RegularChains`. These both produce CADs of real space and there are multiple interesting results to note.

Using PL-CAD behaves much the same as QEPCAD, which is to be expected as both are based on projection and lifting construction of CAD. For six of the ten experiments preconditioning was beneficial, for three the experiment timed out both with and without preconditioning, and for Collision A a previously feasible problem was rendered infeasible by preconditioning. Using the recursive version of CAD via Regular Chains (Section 2.5.2) we get similar results to the other methods discussed so far (seven examples are improved by preconditioning, and three remain infeasible with or without preconditioning).

Problem	PL-CAD		$=_G$-PL-CAD		RC-Rec-CAD		$=_G$-RC-Rec-CAD	
	Cells	Time	Cells	Time	Cells	Time	Cells	Time
Int A	3723	18.885	273	0.897	3723	11.248	273	1.400
Int B	3001	15.272	189	0.528	2795	8.896	189	1.034
Ran A	2101	11.376	165	0.530	1267	5.790	165	0.580
Ran B	7119	73.856	141	0.540	7119	62.182	141	0.531
Ell A	FAIL	T/O	FAIL	T/O	81193	516.385	37789	212.289
Ell B	—	T/O	—	T/O	—	T/O	—	T/O
Sol A	54037	263.054	28501	126.930	54037	329.205	28501	220.144
Sol B	154527	851.669	10633	44.437	154527	1136.397	10633	113.368
Col A	8387	79.006	—	T/O	—	T/O	—	T/O
Col B	—	T/O	—	T/O	—	T/O	—	T/O

Table 6.1: The experiments from [BH91] as rerun with other methods of constructing CADs in Maple. Times are in seconds and "T/O" means a time-out (limit 30mins).

New Data Set

We investigate a new collection of examples using two algorithms: `CADFull` from `ProjectionCAD` (using McCallum's projection operator where possible); and the recursive `CylindricalAlgebraicDecompose` algorithm from `RegularChains` (as released in Maple 16). These represent the projection and lifting approach (Section 2.3), and the original regular chains approach to computing CAD (Section 2.5.2). These algorithms offer the added benefits of providing us with the number of cells computed (a more accurate measurement of CAD complexity than timing) and can all be run (along with the preconditioning stage) within the same `Maple` environment.

Whilst preconditioning is not changing the underlying theoretically minimal CAD, it is changing the way such a CAD can be formed. This is not reliant on the method of construction, so the behaviour should be broadly similar across both algorithms.

Remark 6.1.
Any results given in this thesis for RC-Rec-CAD may differ slightly from those in [WBD12] owing to the use of new implementations of this algorithm[1]. There also may be differences in Maple's implementation of the Gröbner algorithms. We have noted when results have been sourced from [WBD12]; otherwise the results are new and current.

Problem	RC-Rec-CAD		$=_G$-RC-Rec-CAD		Ratio	
	Cells	Time	Cells	Time	Cells	Time
Cyclic-3	381	3.136	21	0.265	18.14	11.83
Cyclic-4	—	$> 1000s$	621	5.877	—	—
CMXY 2	895	2.249	579	1.867	1.55	1.20
CMXY 4	421	3.225	1481	19.762	0.28	0.16
CMXY 6	41	0.363	89	0.938	0.46	0.39
CMXY 7	895	3.667	1211	6.563	0.74	0.56
CMXY 8	365	3.216	51	0.195	7.16	16.49
CMXY 13	4949	14.342	81	0.238	61.10	60.26
CMXY 14	27551	334.860	423	0.992	65.13	337.56

Table 6.2: Examples of Gröbner preconditioning sourced from [CMXY09]. Times are given in seconds and the results are those published in [WBD12].

$=_G$ with CAD

We investigate the effect of $=_G$ (following from [BH91]) and $\rightarrow_G^*$ on a collection of new examples sourced from [CMXY09], along with the Cyclic-3 and Cyclic-4 examples. The CADs are constructed using the recursive regular chains CAD. We see similar behaviour, with some substantial savings, but note there are three examples where preconditioning is detrimental: the worst case increases cell count from 421 to 1481.

$=_G$ with Complex Decompositions

As described in Section 2.5.2, to construct a CAD using regular chains methods a complex decomposition is first constructed. This complex decomposition is then converted to a CAD of real space using the `MakeSemiAlgebraic` command. Table 6.3 shows the effect that Gröbner preconditioning has on these two steps when considering the original examples from [BH91]. In Table 6.3 we use $\mathbb{C}$-CD to denote the complex decomposition algorithm used in RC-Rec-CAD (the `ComplexDecomposition` procedure in the `RegularChains` package in Maple) and `MSA` to denote the `MakeSemiAlgebraic` stage. The ratio listed is between the $\mathbb{C}$-CD and `MakeSemiAlgebraic` columns.

It is interesting to note that preconditioning affects both the complex decomposition and `MakeSemiAlgebraic` stages of RC-Rec-CAD construction. This is perhaps not surprising: Gröbner preconditioning simplifies the representation of the polynomial ideal over *complex* space, and so the complex decomposition should be simpler and easier to compute. This will have a cumulative effect during the conversion to a CAD of real space.

[1]The `ProjectionCAD` package was not developed when [WBD12] was published and so any results for PL-CAD are new.

Problem	$\mathbb{C}$-CD Time	MSA Time	RC-CAD Time	Ratio	$=_G$-$\mathbb{C}$-CD Time	MSA Time	$=_G$-RC-CAD Time	Ratio
Int A	5.691	23.735	29.426	4.17	1.168	1.302	2.470	1.11
Int B	5.584	30.678	36.262	5.49	0.886	0.595	1.481	0.67
Ran A	4.614	12.741	17.355	2.76	0.310	0.260	0.570	0.84
Ran B	67.343	289.327	356.670	4.30	0.318	0.152	0.470	0.47
Ell A*	85.425	177.198	262.623	2.07	27.916	34.580	62.496	1.24
Ell B*	441.245	—	$> 1000s$	—	—	—	$> 1000s$	—
Sol A*	6.666	9.348	16.014	1.40	1.760	0.265	2.025	0.15
Sol B*	9.536	33.903	43.439	3.56	1.404	0.243	1.647	0.17
Col A*	41.085	174.943	216.028	4.26	—	—	$> 1000s$	—
Col B*	—	—	$> 1000s$	—	—	—	$> 1000s$	—

Table 6.3: Examples from [BH91] investigated over the complex numbers with the recursive regular chains algorithms (an asterisk indicates that any inequalities have been omitted to ease CAD construction). Times are given in seconds and the results are those published in [WBD12].

This is supported by the fact that without preconditioning the `MakeSemiAlgebraic` stage is often costly, but this cost is heavily reduced after $=_G$ preconditioning.

Another note of interest is the shift in the division of time between the $\mathbb{C}$-Rec-CD and `MakeSemiAlgebraic` algorithms following preconditioning. Without preconditioning the majority of time is always spent in the `MakeSemiAlgebraic` phase and this is often a significant portion (nearly 5.5 times the time taken for the complex decomposition in Intersection B). Following preconditioning this is no longer true, with only two out of seven examples taking longer to convert the complex decomposition into a CAD (with the worse case being only a ratio of 1.24). This is often quite a shift (Intersection B changes ratio from 5.49 to 0.67) and it would be of interest to investigate this behaviour further.

$\rightarrow_G^*$ with CAD

We wish to investigate the effect of $\rightarrow_G^*$. Consider the following four spheres in $\mathbb{R}^3$:

$$S_1: \quad (x-1)^2+y^2+z^2-3; \qquad S_2: \quad (x+1)^2+y^2+z^2-3;$$
$$S_3: \quad (x-1)^2+(y-\frac{1}{2})^2+z^2-3; \quad S_4: \quad (x+1)^2+(y+\frac{2}{3})^2+(z+\frac{3}{4})^2-3.$$

Define the infinite cylinder centred on the z-axis with radius 1 to be C, so that the equation defining C is:

$$C: \quad x^2+y^2-1.$$

Spheres	PL-CAD A		PL-CAD B		$=_G$-CAD A		$=_G$-CAD B		$\rightarrow^*_G$-CAD A		$\rightarrow^*_G$-CAD B	
	Cells	Time	Cells	Time	Cells	Time	Cells	Time	Cells	Time	Cells	Time
{ }	13	0.053	13	0.030	—		—		—		—	
{1}	617	2.190	123	0.506	617	2.176	123	0.512	71	0.257	123	0.517
{2}	617	2.104	123	0.438	617	2.110	123	0.494	71	0.220	123	0.478
{3}	1109	4.306	173	0.833	1109	4.430	173	0.846	351	1.555	173	0.863
{4}	1401	5.481	173	0.997	1401	5.543	173	0.891	351	1.535	173	0.991
{1, 2}	1073	4.156	631	2.513	267	0.795	171	0.353	99	0.230	99	0.206
{1, 3}	9859	53.507	897	4.820	783	2.274	195	0.533	141	0.476	75	0.206
{1, 4}	10817	62.232	2999	17.407	1439	4.976	315	1.244	213	0.853	249	1.030
{2, 3}	12097	67.623	1317	7.001	1299	3.888	227	0.802	213	0.638	99	0.253
{2, 4}	9051	51.918	1679	9.821	919	3.026	219	0.854	141	0.542	141	0.471
{3, 4}	11957	75.832	3089	18.264	1359	4.781	315	1.259	213	0.841	249	1.010
{1, 2, 3}	23691	138.355	4673	27.607	165	0.398	305	0.468	45	0.096	45	0.054
{1, 2, 4}	21999	138.096	11359	68.513	237	0.844	249	0.666	63	0.160	63	0.132
{1, 3, 4}	62847	479.794	16601	110.485	787	2.298	225	0.748	63	0.250	63	0.146
{2, 3, 4}	64343	544.725	14845	111.714	939	3.012	225	0.780	63	0.173	63	0.165
{1, 2, 3, 4}	140309	1226.077	53509	438.107	13	0.027	13	0.030	1	0.007	1	0.002

Table 6.4: Results of experimentation with Gröbner preconditioning (both $=_G$ and $\rightarrow^*_G$) on examples involving spheres and a cylinder using PL-CAD (`CADFull` from `ProjectionCAD` with the McCallum projection operator).

We consider the intersection of spheres in relation to the cylinder and consider all possible combinations, with some 'simpler' (with regards to the projection structure needed for CAD) than others. We use two variable orders: $z \prec y \prec x$ and $x \prec y \prec z$, which we denote by A and B respectively. The latter variable ordering is arguably the more suitable for these examples: the cylinder C gets projected down to a unit circle in (x, y)-space.

We will assume that the spheres will always be required to equal 0, but make no assumptions on the condition for the cylinder. All problems will therefore be of the form:

$$\bigwedge_{i \in \mathcal{I}} S_i = 0 \wedge C * 0 \qquad \mathcal{I} \subseteq \mathcal{P}(\{1, 2, 3, 4\}), \quad * \in \{=, \neq, <, >, \leq, \geq\}.$$

and we denote such a problem as *Spheres* $\mathcal{I}$. These problems are therefore naturally suited to both $=_G$ and $\rightarrow^*_G$ forms of Gröbner preconditioning.

Table 6.4 shows the results of preconditioning for these examples when using PL-CAD with the McCallum projection operator.

These results show a wide variety of features of Gröbner preconditioning. Considering just $=_G$, we see that preconditioning is always beneficial when taking a non-trivial basis (two or more polynomials). Moreover, the effect of the preconditioning is usually greater with more polynomials: the size ratio of the preconditioned CAD compared to the original CAD is more pronounced. This is as the Gröbner basis is describing the intersection of the polynomials, which can only reduce in size with the inclusion of more polynomials (although the description of this intersection may be more complicated).

The results from the preconditioning by $\rightarrow_G^*$ are also uniformly beneficial. In most cases it reduces the number of cells significantly, and it never increases the complexity of the CAD. Remarkably, it reduces every CAD to under 400 cells and with *Spheres* $\{1, 2, 3, 4\}$ it reduces 140309 cells to just a single cell.

When considering all four spheres, computing a Gröbner basis identifies that there are no common solutions and so $=_G$-PL-CAD produces a CAD with only 13 cells corresponding to the cylinder, identical to the CAD of *Spheres* { } (note that as the cylinder does not contain z, this is actually a CAD of (x, y)-space uniformly extended in the z-direction). When also using $\rightarrow_G^*$ the cylinder is reduced with respect to the trivial ideal, $\langle 1 \rangle$, and so vanishes: the result CAD is the trivial one consisting of a single cell that encompasses all of $\mathbb{R}^3$.

Monomial Ordering

Note that we have chosen to do our preconditioning with respect to the *compatible* monomial ordering, $\prec_{\text{lex}}$: if the Gröbner basis contains univariate polynomials then they will be in the variable corresponding to the one-dimensional induced CAD. This property indicates that either this ordering or its reverse ($\prec_{\text{ilex}}$) would be the most structured for preconditioning.

In [WBD12] it is shown comprehensively that the compatible ordering, $\prec_{\text{lex}}$, is a better choice compared to the reverse ordering, ($\prec_{\text{ilex}}$). The reverse ordering is never more beneficial than the compatible ordering, and for all examples from [BH91] it renders the examples infeasible.

6.2.4 Heuristics for Gröbner preconditioning

For a given problem involving a conjunction of equations, we have seen there is a choice of whether to apply Gröbner preconditioning ($=_G$ or $\rightarrow_G^*$) and in the previous section it was shown that this is a significant choice. To make this decision, we wish to identify a metric or heuristic that closely correlates with the effect of preconditioning.

Previous Metrics: `td*/td` and `sotd*/sotd`

We have seen in this thesis that `sotd` (Definition 2.42) from [DSS04] can be effective at selecting a variable ordering for CAD. In [DSS04] the authors also considered the total degree metric, `td`, defined to be $\sum_{f \in \mathbf{PROJ}(F)} \deg(f)$.

In [DSS04] the authors discarded `td` as a metric by observing its correlation with `sotd` and noting that `sotd` favours sparse polynomials. It is natural to investigate `td`

Problem	RC-Rec-CAD				$=_G$-RC-Rec-CAD			
	`td*/sotd*`	`td/sotd`	Cells	Time	`td*/sotd*`	`td/sotd`	Cells	Time
$S\ \{1,2\}$	6/18	26/46	1073	8.654	5/9	11/5	267	0.905
$S\ \{2,3\}$	6/19	84/151	12097	189.202	5/11	19/28	1299	5.911
$S\ \{3,4\}$	6/21	96/239	11957	248.340	5/15	23/49	1359	8.159
$S\ \{1,2\} \rightarrow_G^*$	6/18	26/46	1073	8.654	5/7	7/9	99	0.270
$S\ \{2,3\} \rightarrow_G^*$	6/19	84/151	12097	189.202	5/10	11/18	213	0.499
$S\ \{3,4\} \rightarrow_G^*$	6/21	96/239	11957	248.340	5/15	11/28	213	0.580
Int A	6/14	36/82	3763	29.426	17/50	21/47	273	2.470
Int B	6/14	34/84	2795	36.262	15/41	16/32	189	1.482
Ran A	9/16	51/104	1219	17.355	19/68	25/88	165	0.570
Ran B	9/16	98/259	7119	356.670	19/73	25/88	141	0.470
Ell A*	6/24	49/123	28557	262.623	6/26	43/97	14439	62.496
Ell B*	6/24	261/595	—	$> 1000s$	25/253	169317/649367	—	$> 1000s$
Sol A*	10/25	16/36	1751	16.014	10/28	10/21	297	2.025
Sol B*	10/25	21/41	6091	43.439	21/69	19/52	243	1.647
Col A*	6/23	96/295	7895	216.028	27/251	8813/45708	—	$> 1000s$
Col B*	6/23	697/4218	—	$> 1000s$	36/875	75078/1909317	—	$> 1000s$
Cyc-3	6/12	27/44	381	3.136	6/12	7/14	21	0.265
Cyc-4	10/28	141/252	—	$> 1000s$	27/64	32/48	621	5.877
CMXY 2	5/8	14/20	895	2.249	10/17	13/20	579	1.867
CMXY 4	5/12	33/65	421	3.225	16/51	67/137	1481	19.762
CMXY 6	7/21	19/54	41	0.363	25/113	38/154	89	0.938
CMXY 7	7/10	17/25	895	3.667	17/29	21/33	1211	6.563
CMXY 8	4/10	17/48	365	3.216	7/31	13/39	51	0.195
CMXY 13	6/10	23/32	4949	14.342	4/4	4/4	81	0.238
CMXY 14	6/14	6/14	27551	334.860	6/17	6/17	423	0.992

Table 6.5: Experiments showing `td*`, `td`, `sotd*` and `sotd` alongside CAD complexity. Times are given in seconds and these results are partly published in [WBD12].

and `sotd` with respect to Gröbner preconditioning. Using the idea that `sotd` can be used greedily (and so is useful even at a single level of polynomials), it also seems worthwhile to consider the `td` and `sotd` of just the set of input polynomials and corresponding Gröbner basis (rather than their whole projection sets). We denote this simplified use of the metrics by `td*/sotd*`.

Table 6.5 gives the computed `td*`, `td`, `sotd*` and `sotd` values alongside the computation data for examples considered in this chapter. The first results in Table 6.5, from the Spheres examples, look promising: all four metrics correlate to the improvement of preconditioning. Both `td` and `sotd` (and partly `sotd*`) are also able to indicate the further improvement of $\rightarrow_G^*$.

However, the other results show that all four metrics are not aligned to the effect of Gröbner preconditioning. In all ten examples from [BH91] (and all but one sampled example from [CMXY09]) using Gröbner preconditioning causes `td`$*$ to increase or remain constant, and `sotd`$*$ strictly increases, often by a great amount. This is in complete contradiction to the results, where most examples see a sharp drop in complexity. The

two more complex metrics, `td` and `sotd`, perform better but still have flaws: they are tricked by examples such as Solotareff B and CMXY 14.

These results will be more closely investigated in Section 6.2.6.

6.2.5 Total Number of Indeterminates: `TNoI` and `TNoIF`

When we apply Gröbner basis preconditioning to a problem, we are in some sense trying to simplify the set of equations. There is a process similar to variable elimination happening, with equations in few variables being preferable to those with many. With this is mind, it seems sensible to consider the number of variables present in each polynomials of a given problem, which inspires the following definition.

Definition 6.6.
Let F be a set of polynomials and for a polynomial $f \in F$ let $\texttt{NoI}(f)$ be the number of indeterminates present in the polynomial (e.g. $\texttt{NoI}(z - x^2y) = 3$). Then define the **total number of indeterminates** of F, $\texttt{TNoI}(F)$, to be:

$$\texttt{TNoI}(F) = \sum_{f \in F} \texttt{NoI}(f).$$

The `TNoI` of the problems considered in this chapter is given in Table 6.6, showing a promising correlation to the benefit of Gröbner preconditioning. In particular the following three points are of note regarding $=_G$:

1. In the 15 cases where applying $=_G$ reduces `TNoI` there is a significant benefit to preconditioning.

2. In the remaining 7 cases where `TNoI` increases from $=_G$ preconditioning it is generally detrimental to precondition (with one false positive).

3. `TNoI` is not a measure of abstract difficulty of CAD construction.

It is clear from point 3 above that calculating `TNoI` alone is not of huge use, and that something related to the difference or ratio of `TNoI` would be more appropriate. The difference or ratio alone does not predict the improvement to expect, but taking the logarithm of the ratio (equivalently the difference of the logarithms) of `TNoI` is more interesting. This investigated in Section 6.2.6.

Inspired by [DSS04] we also consider the following metric:

Definition 6.7.
For a set of polynomials, F, define the **full total number of indeterminates** of F,

Problem	RC-Rec-CAD				$=_G$-RC-Rec-CAD			
	TNoI	TNoIF	Cells	Time	TNoI	TNoIF	Cells	Time
$S\ \{1,2\}$	8	42	1073	8.654	5	24	267	0.905
$S\ \{2,3\}$	8	93	12097	189.202	6	30	1299	5.911
$S\ \{3,4\}$	8	105	11957	248.340	7	39	1359	8.159
$S\ \{1,2\} \rightarrow_G^*$	8	42	1073	8.654	4	15	99	0.270
$S\ \{2,3\} \rightarrow_G^*$	8	93	12097	189.202	6	15	213	0.499
$S\ \{3,4\} \rightarrow_G^*$	8	105	11957	248.340	7	15	213	0.580
Int A	8	54	3763	29.426	7	24	273	2.470
Int B	8	48	2795	36.262	7	21	189	1.482
Ran A	9	57	1219	17.355	5	15	165	0.570
Ran B	9	87	7119	356.670	5	15	141	0.470
Ell A*	7	150	28557	262.623	6	135	14439	62.496
Ell B*	7	585	—	$> 1000s$	21	112685	—	$> 1000s$
Sol A*	9	36	1751	16.014	8	28	297	2.025
Sol B*	9	56	6091	43.439	7	28	243	1.647
Col A*	7	148	7895	216.028	18	6248	—	$> 1000s$
Col B*	7	464	—	$> 1000s$	22	10848	—	$> 1000s$
Cyc-3	9	39	381	3.136	6	15	21	0.265
Cyc-4	16	164	—	$> 1000s$	6	56	621	5.877
CMXY 2	7	45	895	2.249	14	40	579	1.867
CMXY 4	6	33	421	3.225	11	57	1481	19.762
CMXY 6	4	10	41	0.363	5	12	89	0.938
CMXY 7	8	45	895	3.667	22	55	1211	6.563
CMXY 8	6	24	365	3.216	5	15	51	0.195
CMXY 13	9	72	4949	14.342	4	16	81	0.238
CMXY 14	11	15	27551	334.860	9	15	423	0.992

Table 6.6: Experiments showing TNoI and TNoIF alongside CAD complexity. Times are given in seconds and these results are partly published in [WBD12].

TNoIF(F), to be:

$$\texttt{TNoIF}(F) = \sum_{i=1}^{n} \sum_{f \in F_i} \texttt{TNoI}(f),$$

where the F_i are the successive projection sets for a pre-determined projection operator.

Table 6.6 also includes the data for TNoIF alongside TNoI. We can make a direct comparison to how TNoI predicts preconditioning and notice three points:

1. TNoIF behaves almost identically to TNoI.
2. The false positive for TNoI (CMXY 2) is no longer a false positive for TNoIF.
3. TNoIF was of little use in predicting whether $\rightarrow_G^*$ following $=_G$ was useful for the *Spheres* examples.

Overall `TNoIF` seems a better metric than `TNoI`, although the fact that it did not identify the substantial benefit of preconditioning for CMXY 14 is disconcerting. Whether the added benefit of `TNoIF` outweighs the additional cost of computing the full projection set (which can be costly in complicated examples such as Ellipse or Collision) is debatable and is discussed further in Section 6.2.6.

6.2.6 Statistical Analysis of Heuristics

We now give a statistical analysis of the behaviour of the six metrics: `td*`, `td`, `sotd*`, `sotd`, `TNoI`, `TNoIF`. We give graphical evidence of the degree of their correlation followed by analysis of their sample correlation coefficients. All of these are given with respect to the logarithm of the ratios of the data, as suggested by point 3 of the analysis of `TNoI`.

Recall that the **sample correlation coefficient** between two sets of data X and Y is defined to be:

$$r_{X,Y} = \frac{\sum_{i=1}^{n} \left(X_i - \overline{X}\right) \cdot \left(Y_i - \overline{Y}\right)}{\sqrt{\sum_{i=1}^{n} \left(X_i - \overline{X}\right)^2} \cdot \sqrt{\sum_{i=1}^{n} \left(Y_i - \overline{Y}\right)^2}}.$$

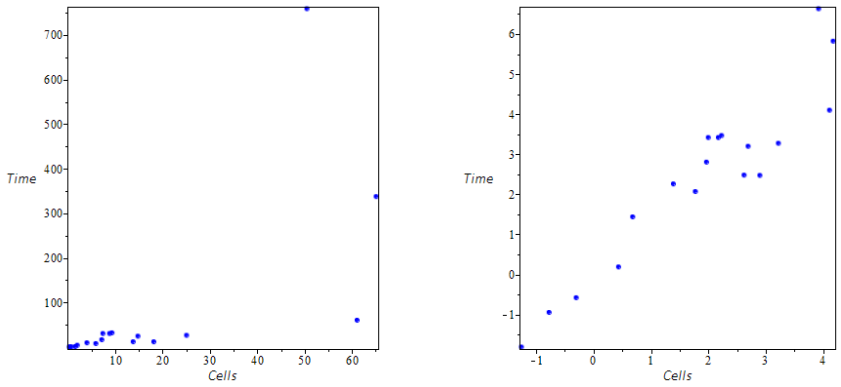
The correlation coefficient is a number between -1 and 1 and indicates the degree of correlation between X and Y: a coefficient of 1 indicates perfect positive correlation; a coefficient of -1 indicates perfect negative correlation; and a coefficient of 0 indicates no correlation between the data sets.

We begin by considering cell counts and time. Figure 6.1 illustrates the standard assumption that the number of cells in a CAD is closely (positively) correlated with the time taken to construct the CAD. This corroborates the findings in [DSS04] and vindicates our decision to often concentrate solely on cell counts (which is unaffected by the hardware used for experimentation). If we perform a linear regression on the logarithmic data we obtain the line $1.27x + 0.03$ which suggests a near-linear correlation.

We now consider the metrics derived from [DSS04] and the new metric `TNoI` in all forms: `td*`, `td`, `sotd*`, `sotd`, `TNoI`, and `TNoIF`. In Figure 6.2, the red circles represent the metric on the input only (`td*`, `sotd*`, `TNoI`) and the blue boxes represent the metric on the full projection set (`td`, `sotd`, `TNoIF`) using the McCallum projection operator.

Figure 6.2a shows the lack of correlation between `td`$*$ or `td` with cell count for the examples considered. Figure 6.2b gives the same for `sotd`$*$ and `sotd`. Figure 6.2c shows that `TNoI` and `TNoIF` both seem comparatively well-correlated with cell count.

We have a limited data set (the 18 examples that completed construction both with and without preconditioning) but the correlation coefficients shown in Table 6.7 give a



(a) Time against cell count.

(b) Log time against log cell count.

Figure 6.1: Graph illustrating the correlation of the ratios of time and cell count.

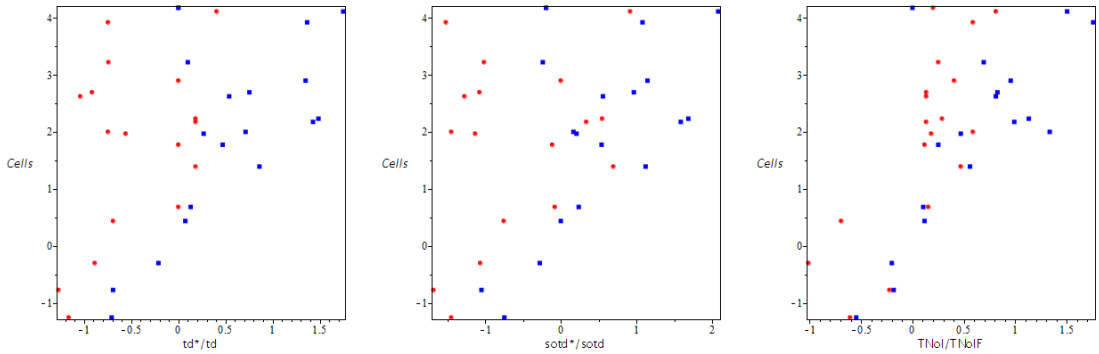
quantitative indication of the results.

As expected, the cell counts and construction time are very strongly positively correlated. Both `td*` and `sotd*` perform poorly, with neither indicating much correlation to the complexity measures. The two more complex measures, `td` and `sotd`, perform better than their simpler counterparts.

It is a little surprising that `td*` and `td` perform better than their respective `sotd*` and `sotd`: total degree is a coarser metric that was dismissed by [DSS04] due to its apparent correlation to `sotd`. It seems this is not the case for Gröbner preconditioning: Gröbner bases can take sparse polynomials and produce quite dense polynomials, which would increase `sotd*` and `sotd` without necessarily increasing `td*` or `td`. For an example of this, computing a Gröbner basis of $\{y^n - 1, xy + x + 1\}$ with respect to either variable ordering produces a fully-dense univariate polynomial of degree $n - 1$ with n terms (e.g. $(y^n - 1)/(y + 1)$). This difference between `td*`/`td` and `sotd*`/`sotd` is worthy of further investigation.

Most importantly, the results show that there is a decent correlation between `TNoI` and `TNoIF` against cell count and construction time. Whilst the correlation is not as strong as the correlation between cell counts and construction time (which is to be expected), it is still significant in all cases. Although working with a relatively small data set, a coefficient greater than 0.75 indicates decent correlation.

What is intriguing is that, unlike `td` and `sotd`, the correlation is slightly worse when the `TNoI` is measured over the whole projection set, as `TNoIF`, rather than just the input. The difference is slight, but contrasts the other metrics where the accuracy doubled



(a) `td*/td` against cell count. (b) `sotd*/sotd` against cell count. (c) `TNoI/TNoIF` against cell count.

Figure 6.2: Graphs illustrating the correlation of the logarithm of the ratio of each metric with cell counts. The red circles indicate `td*/sotd*/TNoIF` and the blue boxes indicate `td/sotd/TNoIF`.

when considering the full projection set in some cases. It is certainly hard to speculate on the reason for this behaviour, but it is perhaps an indication of the fact that `TNoI` was originally invented for use just on input polynomials, whereas `td` and `sotd` were designed for the full projection set.

The correlation coefficients certainly do not tell the full story, and we saw in Section 6.2.5 that `TNoIF` avoids a false positive that `TNoI` misidentifies. However, as the behaviour is so similar in most cases (and the correlation coefficients are so close), there is a convincing argument not to consider `TNoIF` due to the cost of computing the full projection set (for Collision B computing the projection set after preconditioning takes around two minutes of computation time). To this extent, we recommend the use of `TNoI`, unless it cannot predict (for example the $\rightarrow_G^*$-preconditioning of the *Spheres* examples) when `TNoIF` can then be consulted.

Of course, looking at statistical correlation does not explain causation, especially working with a relatively small data set, so we shall look more deeply at what `TNoI` (and consequently `TNoIF`) is measuring.

A Decrease in `TNoI`

We have seen that a reduction of `TNoI` after Gröbner preconditioning is a good indicator that the preconditioning will be beneficial. Let us consider what may cause `TNoI` to decrease.

Let F be a set of polynomials in $x_1 \prec x_2 \prec \cdots \prec x_n$ and let G be the corresponding

Correlation	Coefficient
$r_{Cells,Time}$	$= 0.939$
$r_{td*,Cells}$	$= 0.456$
$r_{td,Cells}$	$= 0.692$
$r_{td*,Time}$	$= 0.446$
$r_{td,Time}$	$= 0.677$
$r_{sotd*,Cells}$	$= 0.330$
$r_{sotd,Cells}$	$= 0.609$
$r_{sotd*,Time}$	$= 0.272$
$r_{sotd,Time}$	$= 0.579$
$r_{TNoI,Cells}$	$= 0.770$
$r_{TNoIF,Cells}$	$= 0.743$
$r_{TNoI,Time}$	$= 0.778$
$r_{TNoIF,Time}$	$= 0.754$

Table 6.7: Correlation coefficients for the logarithm of ratios of cell counts, time, and various heuristics (`td*`, `sotd*`, `td`, `sotd`, `TNoI`, `TNoIF`).

(purely lexicographic) Gröbner basis. The following three reasons are ways that `TNoI` may be less for G than F:

1. The number of polynomials in a particular set of variables, $\{x_{i_1}, \ldots, x_{i_\ell}\}$, is decreased. If x_k is the most important variable in this set, then having fewer polynomials can simplify the decomposition of $(x_1, \ldots, x_k)$-space. If constructing CAD by projection and lifting, then this will also reduce the size of all projection sets at or below level k. These effects will then manifest themselves in the overall CAD by simplifying lifting stages, reducing both the number of cells and the time taken to construct the remaining levels.

2. At least one variable is eliminated from a polynomial in F when computing G. If the variable x_k is eliminated from f (that is, when f is reduced during construction of G, x_k is eliminated), then this will have an effect on the CAD constructed. In particular for projection and lifting, p will not be involved in the k^{th} lift: from $(x_1, \ldots, x_{k-1})$-space to $(x_1, \ldots, x_{k-1}, x_k)$-space. If $k < n$ then this simplification will also simplify further lifting stages. This simplification will reduce the cells produced and the time taken to construct the CAD.

3. A polynomial, f, in a large number of variables, say k, is replaced by polynomials $g_1, \ldots, g_j$ $(j > 1)$ each with k_i variables such that $\sum_{i=1}^{j} k_i < k$. If we consider CAD construction (by projection and lifting or by regular chains) then increasing

the number of polynomials will generally increase the number of resultants and discriminants computed. However, these polynomials, as they are in fewer variables, will be involved in fewer levels and so will have a smaller effect on the CAD than the larger polynomial with many variables.

Let us consider this case a little more precisely: through discriminants, coefficients and resultants, f will be involved in k levels of projection and lifting (all variables will be used). Similarly, the g_i will each feature in k_i levels of projection and lifting. Obviously the sets of variables each g_i involves may intersect one another, but at most there will be $\sum_{i=1}^{j} k_i$ distinct variables. Therefore at worst the g_i will feature in $\sum_{i=1}^{j} k_i$ levels of projection and lifting. This is strictly less than the levels that would be involved with f and so, as long as the degrees of the g_i are not excessive, this should be similar to the effect of point 2 and CAD construction will see a benefit.

Of course, in general, there is not simply one reason for the decrease in `TNoI`: there may be many factors at work at once. There may also be increases in `TNoI` that are getting counteracted, which presumably explains the occasional 'false positive' such as CMXY 2 which shows an increase in `TNoI` but an improvement in CAD efficiency.

Also, it is interesting to note `TNoI` does not take into account the degree of the polynomials produced by Gröbner preconditioning. The degree of a Gröbner basis was shown [Yap91] to be, in the worst case, at least:

$$d^{2^{cn}}, \quad \text{with } c \sim 0.5.$$

This makes it more surprising that `TNoI` does so well to predict the effect of preconditioning and suggests, with respect to Gröbner preconditioning at least, variables are more significant than degree (which, of course, agrees with the complexity estimates of CAD discussed in Section 2.6).

These arguments should transfer to justify the use of `TNoIF`, where many of the points discussed (projection set size, elimination of variables throughout projection sets) should directly manifest themselves.

Using metrics with $\rightarrow_G^*$

It is interesting to consider how the metrics align with preconditioning by $\rightarrow_G^*$. The results in Tables 6.5 and 6.6 suggest that all three of the top-level metrics (`td*`, `sotd*` and `TNoI`) behave similarly: there is a reduction from no preconditioning to $\rightarrow_G^*$ precondition-

ing, and only sometimes a reduction from $=_G$ preconditioning to $\rightarrow^*_G$ preconditioning. This aligns loosely with the benefits shown from the preconditioning but is obviously based on a minimal set of examples. The results are clearer with the metrics on the full projection sets (`td`, `sotd`, `TNoIF`) where generally the metric predicts the benefits of $\rightarrow^*_G$, however `sotd` misidentifies *Spheres* $\{1, 2\}$ (`sotd` increases from 5 to 9, whereas the cell counts decreases from 267 to 99).

6.2.7 Mathematical Justification

Gröbner basis preconditioning ($=_G$)

Informally, taking a Gröbner basis of a set of polynomials constructs a 'simple' way of representing the ideal they generate — they exhibit a clear structure and are as reduced (with respect to each other) as possible. However, as exhibited by examples where preconditioning is detrimental, matters are not so simple.

A Gröbner basis will generally remove any redundancies from a set of polynomials. This may involve reducing polynomials with respect to each other, or identifying common factors. Doing so should benefit the construction of a CAD: when using projection-based CAD we would otherwise still be identifying these factors and having simpler polynomials to start with will produce simpler projection sets. This structural simplification will also be produced when creating CADs through complex decompositions (as in [CMXY09] or [CM12]) where resultants and greatest common divisors are computed, although the simplification is not in such an obvious way.

Remark 6.2.
In Maple's implementation of the Gröbner basis algorithm there is no guarantee that the polynomials are reduced with respect to the basis. They are also generally not computed using Buchberger's Algorithm from [Buc65, Buc06] but instead more modern algorithms such as the F4 algorithm or FGLM algorithm [FGLM93] which converts a basis to one of a different monomial order.

We can be a little more precise than the comment in [BH91] that Gröbner bases produce "triangularized" formulae. Let G be a purely-lexicographical (with $x_1 \prec x_2 \prec \cdots \prec x_n$) Gröbner basis of a *zero-dimensional ideal*. Then G has the form:

$$
\begin{aligned}
G_1 : &\quad p_1(x_1) \\
G_2 : &\quad p_{2,1}(x_1, x_2), \ldots, p_{2,k_2}(x_1, x_2) \\
\ldots &\quad \ldots \\
G_n : &\quad p_{n,1}(x_1, \ldots, x_n), \ldots, p_{n,k_n}(x_1, \ldots, x_n)
\end{aligned}
$$

where $\deg_{x_i}(p_{i,j}) \leq \deg_{x_i}(p_{i,j+1})$ and p_{i,k_i} is monic in x_i [Dav14, §3.3.7]. It seems clear that a set of polynomials in this form would be ideal for CAD construction by projection and lifting.

Denote the set of polynomials in G of level k by G_k. Then in the first round of projection (eliminating x_n) only the polynomials in G_n are used to compute coefficients, discriminants and resultants. In general, when eliminating x_k the polynomials from G_k along with those generated by earlier projections of $G_{k+1}, \ldots, G_n$ are used (and the polynomials in $G_1, \ldots, G_{k-1}$ are disregarded). If we are dealing with a set of polynomials that have not been preconditioned then the set is unlikely to have this structure. Therefore more polynomials are likely to have variables at a high level and so influence the entire projection process.

This discussion is only for zero-dimensional ideals, but it explains why a purely lexicographical monomial order is of use. When an ideal has positive dimension then it may have part of this structure, with stratification across levels of polynomials, but in not quite as strict a way (see Example 6.1).

An interesting question is why Gröbner basis preconditioning is not universally beneficial. When trying to find the 'simplest' way to represent a polynomial ideal, a Gröbner basis might produce extra polynomials of possibly high degree. In [MR10] the authors show that an upper bound on the total degree of a Gröbner basis of a set of polynomials with maximum total degree d defining an r-dimensional ideal in n variables is:

$$
\leq 2\left(\frac{1}{2}d^{n-r} + d\right)^{2^r}.
$$

Further, we know from [Yap91], there exists a set of polynomials of degree bounded by d for which a Gröbner basis will include a polynomial of degree at least:

$$
d^{2^{cn}}, \quad \text{with } c \sim 0.5.
$$

Therefore a Gröbner basis can increase the number and degree of polynomials sub-

stantially (up to a doubly exponential factor), which will increase the complexity and cost of constructing a CAD due to a large increase in the number and degree of resultants and discriminants computed (and the extra cells that they would subsequently define).

It is worth noting that when a Gröbner basis is computed, it is done so with respect to the *complex* ideal for the polynomials. It does not distinguish between the real and complex solutions. This means that the 'simplified structure' will be as viewed over the complexes which may have ramifications over the reals. Obviously a perfect preconditioning method would work over the reals instead, which would eliminate solutions over the complexes. Even though CADs are constructed over the real numbers, complex behaviour can be significant: if we consider the two non-intersecting circles $x^2 + y^2 - 9$ and $x^2 + (y-1)^2 - 1$ then constructing a CAD (with PL-CAD, RC-Rec-CAD or RC-Inc-CAD and $y \prec x$) identifies a spurious point $y = \frac{9}{2}$ which corresponds to a complex intersection of the circles with $x = \frac{\pm 3i\sqrt{5}}{2}$ [Dav11]. Ideally a real-solution inclined preconditioning method would identify that, whilst the y-component of this solution is real, the x-component is complex and so this 'shadow' of a solution would not appear in the CAD.

The issue with preconditioning over the real numbers is that doing so would come much closer to simply solving the problem and so is likely to be much more costly. It would be a worthy research topic to investigate the interaction of triangular decompositions over the reals (for example [CDM$^+$10, Che11]) with CAD. Triangular decomposition may prove useful preconditioning for CADs constructed by regular chains [CMXY09] as they are based on the same technology.

Gröbner reduction preconditioning ($\rightarrow_G^*$)

Now let us consider the further preconditioning of $\rightarrow_G^*$ where inequalities are reduced with respect to the Gröbner basis. It is worth noting that this is not restricted to simply Gröbner bases: any equational constraint, $f = 0$, can be used to reduce other polynomials in a CAD problem as the only solutions that we care about are when f vanishes, and so multiples of f can be added or subtracted to the other polynomials without changing the set of solutions.

Remark 6.3.
Although we do not require a Gröbner basis to apply reduction, it is necessary to ensure a canonical and well-defined complete reduction. For example [Dav14], if $f_1 := x - 1$, $f_2 := x^2$ and $g := x^2 - 1$ then reducing g with respect to $\{f_1, f_2\}$ gives both 0 and -1 depending on which polynomial we chose to use for reduction. However, taking a

Gröbner basis of $\{f_1, f_2\}$ gives the trivial ideal $\langle 1 \rangle$ and so g uniquely reduces to 0.

Consider a set of m polynomials, A, with max degree d, and maximum norm length l. Collins [Col75] showed that the construction of a CAD for A is dominated by:

$$(2d)^{4^{n+4}} m^{2^{n+6}} l^3. \tag{6.6}$$

Now let E be the set of equational constraints ($\{f = 0 \mid f \in E\}$) for the problem (with each $f \in A$) and let $g \in A$ be any non-equational constraint. We assume that E is a Gröbner basis simply to prevent the need to worry about non-unique reductions. Let g^* be the complete reduction of g with respect to E. Then three cases may occur:

$g^* = 0$ If g reduces to 0 then m is reduced by 1, d is possibly reduced (or at worst stays constant), and l is possibly reduced (or at worst stays constant). Therefore the CAD will be dominated by a lower bound.

$g^* \notin \{0, g\}$ In this case then g has been reduced but not fully. Therefore m remains constant and d is possibly reduced (or at worst stays constant). The norm length of g may have increased, and therefore l may have increased. However if there is any change in d then this will greatly outweigh any increase in l (due to the double exponential in d).

$g^* = g$ If g does not reduce at all then m, d and l remain unchanged and therefore so does the complexity bound.

Obviously this discussion is related to an upper bound on the complexity, so the CAD itself may not be simplified. However, any decrease in degree or number of polynomials will simplify the CAD if there is a reduction in the real roots present in the polynomial, its discriminant, or its resultants. If an increase in norm length occurs, this should not affect the constructional complexity of the CAD significantly.

The `TNoI` Metric

We have already discussed in Section 6.2.6 why the `TNoI` (and `TNoIF`) metric may be reduced, and why it is useful for predicting the benefit of Gröbner preconditioning. This aligns with the mathematical justification given in Section 6.2.7 for $=_G$.

In Section 6.2.6, it was discussed briefly how the metrics are loosely aligned with $\rightarrow_G^*$-preconditioning on a small set of examples (with the metrics on the full projection sets being preferable). We now think about the effect this preconditioning would have on the metrics.

When we take the Gröbner normal form of a polynomial we are successively taking the remainder of the polynomial with respect to the Gröbner basis. In doing so, we will potentially reduce the total degree of the polynomial, or the number of indeterminates. However it will potentially increase the number of monomials in a polynomial (by reducing a term in a polynomial by a dense polynomial in the Gröbner basis). Therefore it is possible that `td*`, `td`, `TNoI` and `TNoIF` will remain constant or reduce with $\rightarrow_G^*$-preconditioning, but `sotd*` and `sotd` will increase. We have seen that $\rightarrow_G^*$-preconditioning should be generally beneficial which suggests that `td*`, `td`, `TNoI` and `TNoIF` are better metrics to use than `sotd*` and `sotd`. This is supported by the fact that `sotd` wrongly predicts the effect of $\rightarrow_G^*$-preconditioning on some of the *Spheres* $\{1, 2\}$ examples.

6.2.8 Gröbner preconditioning with EC-CAD and RC-Inc-CAD

Gröbner preconditioning can be combined with other CAD techniques. We will now briefly investigate the effect it has on building CADs with equational constraints and with new CAD algorithms. Later (Section 7.1.2), we will look at preconditioning in relation to TTICADs and other ideas.

Gröbner preconditioning with equational constraints

For $=_G$ preconditioning to be possible, a problem needs to contain a conjunction of at least two equalities in a sub-formula. If these conjuncted equalities occur in the main formula, then all the f_i are also equational constraints. Therefore the equational constraint projection operator and lifting procedure [McC99] can be used to reduce the size of the CAD. We will only consider utilising one equational constraint primarily as the `ProjectionCAD` package does not implement the theory of bi-equational constraints.

Once $=_G$-preconditioning has been applied, then replacing the f_i with the new Gröbner basis means all the $\hat{f}_i$ are equational constraints and eligible for use with equational constraint technology. It seems of interest to investigate if equational constraints are still of use following Gröbner preconditioning and whether they have the same effect.

Table 6.8 shows the effect of $=_G$-preconditioning combined with equational constraint technology. For each example the following are constructed: a standard PL-CAD (using McCallum's projection operator); a $=_G$-preconditioned PL-CAD; an equational constraint PL-CAD with respect to each of the original equational constraints (where 'FAIL' indicates the equational constraint is nullified); an equational constraint PL-CAD with respect to each of the $=_G$-preconditioned equational constraints.

Problem	PL-CAD		$=_G$-PL-CAD		EC-PL-CAD		$=_G$-EC-PL-CAD	
	Cells	Time	Cells	Time	Cells	Time	Cells	Time
Int A	**3723**	**18.885**	**273**	**0.897**	657	2.670	FAIL	—
					463	2.633	FAIL	—
					269	**0.822**	FAIL	—
							195	**0.566**
Int B	**3001**	**15.272**	**189**	**0.528**	711	2.617	FAIL	—
					471	2.936	FAIL	—
					303	**0.724**	FAIL	—
							147	**0.408**
Ran A	**2101**	**11.376**	**165**	**0.530**	**375**	1.785	FAIL	—
					435	2.367	FAIL	—
					425	**1.759**	**165**	**0.624**
Ran B	**7119**	**73.856**	**141**	**0.540**	1295	13.293	FAIL	—
					477	**2.416**	FAIL	—
					1437	15.433	**141**	**0.530**
Ell A	—	T/O	—	T/O	—	T/O	—	T/O
					—	T/O	FAIL	—
Ell B	—	T/O	—	T/O	—	T/O	—	T/O
					—	T/O	FAIL	—
					—	T/O	—	T/O
							—	T/O
Sol A	**54037**	**263.054**	**28501**	**126.930**	FAIL	—	FAIL	—
					FAIL	—	FAIL	—
					20593	**65.443**	FAIL	—
					22109	116.412	**12513**	**53.655**
Sol B	**154527**	**851.669**	**10633**	**44.437**	FAIL	—	FAIL	—
					FAIL	—	FAIL	—
					48475	**172.039**	FAIL	—
					63583	345.607	**4809**	**19.767**
Col A	**8387**	**79.006**	—	T/O	**2999**	**22.152**	FAIL	—
					2999	23.198	FAIL	—
					—	T/O	FAIL	—
							—	T/O
							—	T/O
							—	T/O
Col B	—	T/O	—	T/O	—	T/O	FAIL	—
					—	T/O	—	T/O
							—	T/O
							—	T/O
							—	T/O

Table 6.8: Results of combining Gröbner preconditioning with equational constraints. Examples are sourced from [BH91] and times are given in seconds. FAIL indicates an equational constraint was nullified and so a CAD could not be constructed. T/O indicates a time-out (limit 30 minutes).

There are some interesting things to note from Table 6.8. Comparing the $=_G$-PL-CAD and EC-PL-CAD columns we see that Gröbner preconditioning usually has a stronger effect than equational constraints. However, equational constraints has the added benefit of never being detrimental to CAD construction (the equational constraint projection set is simply a subset of the McCallum projection operator).

When combined, Gröbner preconditioning and equational constraints prove even more powerful. The final column shows that startlingly low cell counts can be obtained for these reasonably difficult problems. As utilising an equational constraint can only be beneficial, this is unsurprising.

What is also unsurprising is that lifting with respect to equational constraints from the Gröbner basis often fails due to nullification on a cell of positive dimension. This is due to the loosely triangular structure that lexicographical Gröbner bases exhibit (as discussed in Section 6.2.7) which results in equational constraints in few variables. As a compatible variable ordering is used, these polynomials with few variables are at a low level (including often, a univariate polynomial in the lowest variable) and so are nullified on positive dimensional cells simply by construction of a sign-invariant CAD.

Gröbner preconditioning with incremental CAD

We now consider constructing CADs incrementally by regular chains [CM12] (Section 2.5.3). One particular advantage of this approach is the ability to easily use all possible equational constraints. In constructing the complex tree for a given problem, refinement with respect to equational constraints allows for all constraints to be used, unlike projection-based techniques.

This has an interesting effect on Gröbner preconditioning. Table 6.9 shows the effect of Gröbner preconditioning on RC-Inc-CAD. Preconditioning seems to alter the constructed CAD to a smaller degree than PL-CAD or RC-Rec-CAD, in part due to the fact multiple equational constraints are being considered.

Consider the first example, Intersection A.

$$x^2 - \frac{1}{2}y^2 - \frac{1}{2}z^2 = 0 \wedge xz + zy - 2x = 0 \wedge z^2 - y = 0.$$

Utilising all the equational constraints will consist of identifying all the points were all three equations are satisfied. The solution set consists of 3 real solutions and the incremental algorithm will identify these three points and build a CAD that identifies just these points. This CAD consists of three planes (parallel to the plane defined by the axes of the two largest variables) intersecting the solution points. Each plane is

Problem	RC-Inc-CAD		$=_G$-RC-Inc-CAD	
	Cells	Time	Cells	Time
Int A	19	0.105	19	0.101
Int B	19	0.102	19	0.092
Ran A	31	0.131	31	0.124
Ran B	31	0.140	31	0.130
Ell A	10395	28.966	10395	31.113
Ell B	67113	399.152	9345	46.292
Sol A	29	0.158	29	0.147
Sol B	33	0.202	33	0.160
Col A	595	3.041	271	1.664
Col B	2803	318.570	—	T/O

Table 6.9: The experiments from [BH91] as rerun with RC-Inc-CAD in MAPLE. Times are in seconds and T/O means a time-out (limit 30mins).

divided by a line through its solution point (parallel to the axis of the main variable), and the solution point divides this line. This results in four three-dimensional cells, six two-dimensional cells, six one-dimensional cells, and the three zero-dimensional cells at the solution points. This gives the smallest possible CAD that is identified by the incremental algorithm.

Applying Gröbner basis preconditioning to the polynomials in the above example does not change the solution set as the Gröbner basis is, by definition, a basis of the ideal defined by the polynomials. Therefore exactly the same CAD is produced by the incremental CAD. This is true of the first four examples.

The latter examples show that Gröbner preconditioning can still be of use when there are non-equational constraints present, although the Solotareff examples show that the presence of non-equational constraints does not guarantee a change when using preconditioning.

Note also that as the behaviour of preconditioning is notably different to that of PL-CAD or RC-Inc-CAD it is likely that `TNoI` or `TNoIF` will not be as effective as heuristics. They should still be of more use than `td*`, `td`, `sotd*`, or `sotd` though, and could still be used to help decide whether to precondition (although this requires further research).

6.2.9 Extensions to the theory

We briefly discuss some interesting extensions to Gröbner preconditioning and potential future research topics.

Phisanbut [Phi11] investigated the application of CAD to branch cuts in the complex plane (discussed in Section 2.8.1). These problems generally contain "half-line" formulae: $f = 0 \wedge g > 0$. These can be pseudo-reduced to $f = 0 \wedge \text{prem}(g, f) > 0$, where prem indicates the pseudo-remainder. To ensure the sign of this pseudo-remainder is the same as g, we must multiply g by an even power of the leading coefficient of f. Phisanbut found that often, but not always, this pseudo-reduction resulted in a significant decrease in the number of cells. It would be interesting to investigate the combination of this preconditioning following the application of $=_G$, and compare to the effect of $\rightarrow_G^*$.

We know that variable ordering is of importance for both CAD construction and Gröbner basis computation. Throughout this chapter we have assumed that the variable ordering has been fixed before considering whether to precondition or not. Obviously a variable ordering may not be fixed (although the choice may be restricted in quantifier elimination problems) and the choice of ordering and preconditioning will likely be dependent on each other. Initial exploratory experiments suggest that the choices are not straightforward: preconditioning may be beneficial with one variable ordering and not with another; the best variable ordering without preconditioning can be different from the best variable ordering with preconditioning. Ideally, one could identify a heuristic that could be used to pick the best choice of variable ordering and preconditioning, but this would not be a small task: a large amount of data would need to be collected (for each problem in n variables, $2(n!)$ experiments would need to be conducted). This is revisited in Chapter 7.

In Table 6.3 the proportion of time spent between creating the complex decomposition and converting it to a RC-Rec-CAD of real space was investigated. There was an interesting shift, with the complex decomposition dominating most examples after preconditioning. It would be interesting to investigate whether this shift still occurs when using RC-Inc-CAD, along with how variable ordering affects these timings.

One of the most promising ideas for heuristics is that of machine learning and in Section 5.3 we discussed the application of machine learning techniques to choose a heuristic for the choice of variable ordering. It seems like Gröbner preconditioning is also well-suited for the application of machine learning. It would be interesting to use machine learning in two ways with Gröbner preconditioning: indirectly making it select a heuristic to use for a given problem (from those heuristics discussed in Section 6.2.4); or directly answering if preconditioning should be applied or not.

6.2.10 Conclusions on Gröbner Preconditioning

In this section we conclusively showed that Gröbner preconditioning for CAD construction is a worthwhile area of study. Taking a Gröbner basis of a conjunction of equalities was shown to be generally beneficial, although there are cases where it can be detrimental to the complexity of the subsequent CAD. Experimental data was backed up by mathematical justification why this may be the case. A metric, `TNoI` (and its generalisation `TNoIF`), was given and it was shown to be well correlated to when preconditioning is beneficial, with mathematical reasons given for this behaviour.

Further preconditioning was given by reducing inequalities with respect to the computed Gröbner basis. Experimentation suggests this is always beneficial (when it is possible) and complexity bounds on CAD support this.

The effect of combining Gröbner preconditioning with other advances in CAD theory was investigated and shown to be beneficial when combined with equational constraints or incremental CAD. Finally, suggestions of how to extend this preconditioning and more accurately predict its effect were briefly discussed.

6.3 Case Study: The Piano Mover's Problem

We demonstrate the benefit of choosing the correct expression of a problem for CAD by considering the **Piano Mover's Problem**[2] of moving an infinitesimally thin piano through a right angled corridor. An expression of this problem was shown in [Dav86] to be infeasible when tackled with CAD and that is still the case 25 years later.

We do not present this section as an argument for using CAD for robotic motion planning. Indeed, the intention of using the Piano Mover's problem is precisely to have a problem that is very difficult for CAD to tackle, and to therefore have a case study of how the mathematical description of a problem can affect the feasibility of using CAD. Further, any motion planning application would not require the solution of a single setting (such as given in this chapter), but repeated computations for different environments with multiple objects. These would need to be solved in essentially real time, which is beyond the scope of CAD.

Various amounts of geometric analysis can offer alternative expressions and we survey the literature demonstrating their effectiveness. These simpler formulations allow CAD

[2]There seems little consistency in the literature with regards to the punctuation of *Piano Mover's*, with instances of *Piano Mover's*, *Piano Movers'*, and *Piano Movers*. All options are valid possibilities, and we use the convention of *Piano Mover's*, corresponding to a singular protagonist (as our piano is infinitely thin, therefore weightless, and so easily carried by one piano mover).

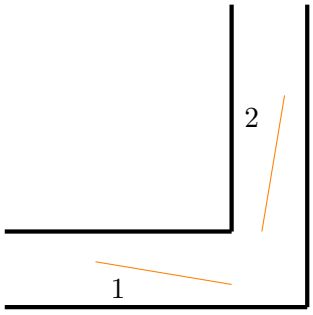


Figure 6.3: The piano mover's problem considered in [Dav86].

to easily address the question of the existence of a path. We do not rely on subtle geometric analysis but produce a new expression for which both a CAD can be constructed and from which an actual path could be determined (if one exists). A comparison of the CADs produced by all methods is given.

The ideas in this section will lead to general ideas about the expression of a problem for CAD which will be discussed in Section 6.4.

All the work in this section is adapted from [WDEB13] which first appeared in the Technical Report [WBDE13].

6.3.1 Introduction to the Piano Mover's Problem

In [SS83b] the authors define the general **Piano Mover's Problem** as: "given a body B and a region bounded by a collection of walls, either find a continuous motion connecting two given positions and orientations of B during which B avoids collisions with the walls, or else establish that no such motion exists." Such a problem can commonly arise in robotics.

A simple example of such a problem was given in [Dav86], where the author considered moving a ladder of length 3 through a right-angled corridor of unit width. This is shown in Figure 6.3 where we wish to move the ladder from position 1 to position 2. A simple geometric analysis shows that with a ladder of length 3 there is no solution to this particular problem: it is only possible to traverse the corridor if the ladder has length less than $\sqrt{8}$. The work in [SS83a, SS83b, Dav86, etc] and continued in [WDEB13] investigates how this and similar piano mover's problems may be decided automatically through CAD, providing a path when a solution exists.

In [SS83b] the authors proposed a generic approach to piano mover's problems in which the problem is described using polynomial algebra and then solved using a CAD algorithm. However, for even very simple examples this approach can be computationally

infeasible. In [Dav86] the author applied this approach to the problem shown in Figure 6.3 and demonstrated that the scale of computations required rendered this approach completely infeasible. Despite 25 years of improvements in CAD theory and computer hardware, creating a CAD with respect to this algebraic formulation is still infeasible.

6.3.2 Original formulation of the problem from [Dav86]

In [Dav86] the author considered building a CAD to solve the problem of moving a ladder of length 3 through a right-angled corridor of width 1 (as in Figure 6.3). Denoting the endpoints of the ladder as (x, y) and (w, z) and assuming the outer corner of the corridor as the origin, the formulation provided was:

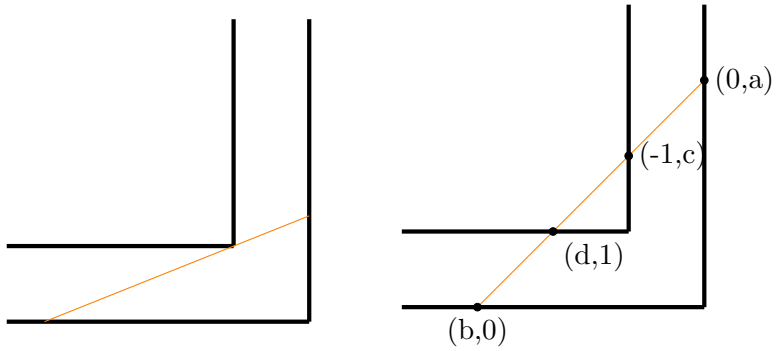
$$\Big[\big[(x-w)^2+(y-z)^2-9=0\big]\wedge \\ \big[[yz\geq 0]\ \vee [x(y-z)^2+y(w-x)(y-z)\geq 0]\big]\wedge \\ \big[[(y-1)(z-1)\geq 0]\vee[(x+1)(y-z)^2+(y-1)(w-x)(y-z)\geq 0]\big]\wedge \\ \big[[xw\geq 0]\vee\ [y(x-w)^2+x(z-y)(x-w)\geq 0]\big]\wedge \\ \big[[(x+1)(w+1)\geq 0]\vee[(y-1)(x-w)^2+(x+1)(z-y)(x-w)\geq 0]\big]\ \Big]. \quad (6.7)$$

The first equation in (6.7) describes the length of the ladder, and the remaining inequalities describe the valid positions, ensuring the ladder does not intersect any of the four walls. In [Dav86] the author completed the projection phase of Collin's CAD algorithm, finding over 250 distinct univariate projection factors with total degree as high as 26. The technology available for the paper did not allow for the simultaneous root isolation of these. With current hardware and software (QEPCAD-B 1.69 and the recursive regular chains CAD algorithm) it still remains outside the realm of computation to complete the construction of the CAD.

6.3.3 Other Approaches in the Literature

We freely acknowledge that in a practical robotic application, the piano mover's problem would typically be tackled using numerical or hybrid methods. This allows for an efficient solution and can even provide exact solutions. We are instead concerned with the symbolic approach to the problem through CAD. We now discuss previous approaches to this problem with CAD in the literature.

The first substantial work on approaching the piano mover's problem symbolically with CAD was [SS83b]. In [SS83a] the same authors had proposed a separate approach



(a) A ladder with endpoints in opposite branches of the corridor.

(b) A ladder for which all four walls are intersected.

Figure 6.4: Important configurations of a ladder in a right-angled corridor.

which did not rely on CAD and was restricted to the plane. This algorithm is typically more efficient than a CAD-based approach, but does not generalise past two dimensions.

The idea of tackling the piano mover's problem with CAD has been considered in various papers. In [Mar89] the author discusses this particular problem and suggests the question of traversing the corridor is equivalent to deciding if there is a position of the ladder for which both extremities are in the two branches of the corridor. This verbal description of his geometric reasoning can be misleading, as Figure 6.4a illustrates a positioning of the latter with endpoints in opposite branches of the corridor but for which the ladder is still unable to turn the corner.

Later in [Mar89] the author gives another expression of this piano mover's problem, which is parameterised by one endpoint and the tangent of the half-angle between the ladder and the x-axis. The author reports that a CAD can be produced for this using Collins' original CAD algorithm and that it is sufficient to conclude that the problem has no solution. No details of the algebraic formulation are provided and we are unable to verify this or analyse this way of formulating the problem further.

In [Wan96], the author uses "simple reasoning" to deduce that the ladder cannot traverse the corridor if and only if it can intersect all four walls simultaneously. This deduction is straightforward (although does not generalise easily) and from this the problem can be expressed in the following manner. Let a, b, c, d be coordinates defining the intersection points as in Figure 6.4b and r be the length of the ladder. Then there

is no solution if and only if:

$$(\exists a)(\exists b)(\exists c)(\exists d)\Big[\left[a^2+b^2=r^2\right]\wedge[r>0]\wedge[a\geq 0]\wedge[b<0]\wedge[c\geq 1]\wedge[d<-1]$$
$$\wedge[c-(1+b)(c-a)=0]\wedge[d-(1-a)(d-b)=0]\Big]. \quad (6.8)$$

As there is only a single free variable, the length r, and the relative simplicity of the formulation QEPCAD can solve the given problem almost instantly, using a partial CAD of 19 cells to state that the maximal length of the ladder is $\sqrt{8}$ (a fact that can be verified with a purely geometric argument). Note also that this problem contains three equational constraints, of which QEPCAD can use the theory of [McC99] to utilise one of these.

In [Wan96], the authors notes that if the ladder intersected both outer walls and one of the inner walls then it must also intersect the other inner wall. Therefore (6.8) can be simplified further by removing the two formulae $[d<-1]$ and $[d-(1-a)(d-b)=0]$. This can be considered further topological reasoning, but does not make a difference in the timing or cell counts from QEPCAD (although such reasoning could be powerful for other problems).

In [McC97] the author approaches path-finding by considering transformations of objects by a translation vector (x,y) and a rotation angle θ (instead of their absolute position in Cartesian space). This produces 21 formulae in a relatively complicated Boolean formula which describes the techniques. McCallum then appeals the theory of equational constraints, partial CAD techniques, parallelisation and a form of sub-CAD (described in Section 4.1.1) to construct a four-dimensional sub-CAD consisting of 16138 cells in 429 seconds.

In [YZ06] the authors looked at a two-dimensional rectangular piano, instead of the one-dimensional ladder. They use geometric analysis to produce a simple condition for the problem to have a solution. They describe the problem according to the position of a particular corner of the rectangle and the angle the rectangle makes with the horizontal axis. They allow for the corridors to have non-unit (and non-equal) widths (denoted a and b) and include the length and width of the rectangle (denoted L and r) as two other parameters. They then provide, through some highly non-trivial analysis, a positive definiteness condition on a degree 8 polynomial involving these four parameters and a single variable x: if this condition holds, then a valid route exists. Reducing the problem to the ladder in Figure 6.3 with the ladder having length L, their reasoning states that

the existence of a valid route is equivalent to the truth of the following Tarski formula:

$$(\forall x)\ \left[4x^8 - 4(L-3)x^6 - 2(3L-6)x^4 - 2(L-3)x^2 + 1 > 0\right].$$

As this is a single polynomial in two variables (one of which is quantified) it takes QEPCAD just 1.936 seconds (mostly initialisation time), and a partial CAD containing only 5 cells, to return the equivalent formula

$$\Big[\left[L^2 - 8 < 0\right] \vee \left[L < 0\right]\Big].$$

Although the approaches of [Wan96, YZ06] are highly efficient, they are also limited. They require (especially in the case of [YZ06]) significant geometric deductions before they use any CAD technology. Further, they can only answer whether the ladder can traverse the corridor successfully, without information about what a successful path could be. This approach could therefore be used as an initial way of deciding whether a path is possible, thereafter a necessarily more-complicated CAD could be constructed which would be sufficient for constructing a path.

The geometric approaches give descriptions in the real space describing the geometry of the plan in which the ladder exists. In contrast, the approaches in [SS83b, Dav86] and the new formulation we will give in 6.3.4 describe the geometry in a four-dimensional configuration space: the coordinates of the two endpoints of the ladder within the plane. This is an important distinction: working in a configuration space allows the constructed CAD to be used to construct an explicit path, whereas a CAD of the real space can only analyse if a ladder can move through the corridor or not.

The configuration space also allows us to consider further properties such as the orientation of the ladder. The descriptions given in [Wan96] and [YZ06] cannot distinguish whether the ladder is able to rotate within the corridor and exit in the reverse orientation to its entry. This is an important point for generalisations of this problem, including those discussed in Section 6.3.8.

The description of the problem in [McC97] is also within a configuration space, although a different non-trivial one where positions are encoded through transformations.

6.3.4 New Formulation of the Problem

We now consider the problem from a different perspective within the same configuration space as in [Dav86]. We describe all the possible invalid regions and then take their negation to describe the valid regions. As in (6.7) we denote the positions of the endpoints

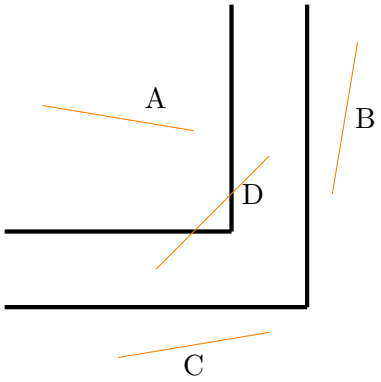


Figure 6.5: Four canonical invalid positions of the ladder. For positions A–C only one end needs to be outside the corridor.

of the ladder by (x, y) and (w, z).

We break down this process to give the most clarity to the method.

Describing the invalid regions

There are four canonical invalid configurations of the ladder, and an example of each is shown in Figure 6.5. Each invalid positioning can be described by an equivalent formula:

A: $x < -1 \wedge y > 1$ or $w < -1 \wedge z > 1$ — this describes any collision with the 'inside' walls along with the ladder being entirely on the inside of these (like ladder A is positioned in Figure 6.5).

B: $x > 0$ or $w > 0$ — this describes any collision with the rightmost wall along with the ladder being entirely to the right of this wall (like ladder B is positioned in Figure 6.5).

C: $y < 0$ or $z < 0$ — this describes any collision with the bottommost wall along with the ladder being entirely below this wall (like ladder C is positioned in Figure 6.5).

D: $(\exists t)[0 < t \wedge t < 1 \wedge x + t(w - x) < -1 \wedge y + t(z - y) > 1]$ — this ensures no inner point of the ladder lies in the invalid top-left region (like ladder D is positioned in Figure 6.5).

We can hence characterise the invalid regions as:

$$(\exists t)\Big[\,[x < -1 \wedge y > 1] \vee [w < -1 \wedge z > 1] \vee [x > 0] \vee [w > 0] \vee [y < 0] \\ \vee [z < 0] \vee [0 < t \wedge t < 1 \wedge x + t(w - x) < -1 \wedge y + t(z - y) > 1]\,\Big]. \quad (6.9)$$

The formula (6.9) contains the new quantified variable t used to parametrise the points on the ladder. We can use QEPCAD to eliminate t from (6.9) in just over 2 seconds (including initialisation). The partial CAD constructed contains 681 cells and the following quantifier-free formula is returned:

$$\Big[[y<0]\vee[w>0]\vee[x>0]\vee[z<0]$$
$$\vee[x+1<0\wedge y-1>0]\vee[w+1<0\wedge z-1>0]$$
$$\vee[w+1<0\wedge yw-w+y+x\geq 0\wedge xz+z-yw+w-y-x>0]$$
$$\vee[yw-w+y+x<0\wedge z-1>0\wedge xz+z-yw+w-y-x<0]$$
$$\vee[y-1>0\wedge yw-w+y+x<0]\Big]. \quad (6.10)$$

Note that we could use QEPCAD to eliminate the spurious variable t from the final formula in (6.9) alone (just the formula describing case D). This constructs 1063 cells and takes only 0.2 seconds to return an equivalent answer (once conjoined to the remaining conditions A–C) to (6.10). This is quicker but produces more cells than (6.9) as it cannot take full advantage of QEPCAD's in-built tools (such as partial CAD and formula simplification).

New formulation for CAD

We therefore have a complete description of the invalid positions of the ladder, (6.10), so we can describe the valid regions by taking its negation:

$$\Big[[w\leq 0]\wedge[x\leq 0]\wedge[y\geq 0]\wedge[z\geq 0]\wedge[x\geq -1\vee y\leq 1]\wedge[w\geq -1\vee z\leq 1]$$
$$\wedge\big[wy-w+x+y<0\vee w+1\geq 0\vee xz+z-yw+w-y-x\leq 0\big]$$
$$\wedge\big[yw-w+y+x\geq 0\vee[[z-1\leq 0\vee xz+z-yw+w-y-x\geq 0]\wedge y-1\leq 0]\big]\Big]. \quad (6.11)$$

We now have, in (6.11), a complete description of the valid regions in terms of the endpoints. The only thing left to completely describe the Piano Mover's Problem is the relationship between the endpoints, which in this example is the equation fixing the length of the ladder. Hence our new formulation for the Piano Mover's Problem is:

$$[(x-w)^2+(y-z)^2=9]\wedge(6.11). \quad (6.12)$$

6.3.5 Applying CAD to the New Formulation

We can input (6.12) to QEPCAD with the standard initialisation parameters (`+N500000000 +L200000`) and variable ordering $x \prec y \prec w \prec z$. After a little under 5 hours (16933.701 seconds) of computation time a CAD of $\mathbb{R}^4$ was constructed with 285419 cells. The following was the output, which is an equivalent formula to (6.12):

$$\begin{gathered}
x \leq 0 \wedge y \geq 0 \wedge w \leq 0 \wedge z \geq 0 \wedge (y-z)^2 + (x-w)^2 = 9 \wedge \\
\Big[[x+1 \geq 0 \wedge w+1 \geq 0] \vee \big[y-1 \leq 0 \wedge w+1 \geq 0 \wedge y^2w^2 - 2yw^2 + x^2w^2 + \\
2xw^2 + 2w^2 - 2xy^2w + 4xyw - 2x^3w - 4x^2w - 4xw + x^2y^2 - 2x^2y + x^4 + \\
2x^3 - 7x^2 - 18x - 9 \geq 0 \big] \vee \big[x+1 \geq 0 \wedge yw - w + y + x \geq 0 \wedge \\
w^2 - 2xw + y^2 - 2y + x^2 - 8 > 0 \wedge z - 1 \leq 0 \big] \vee \big[x+1 \geq 0 \wedge yw - w + y + x \geq 0 \wedge \\
y^2w^2 - 2yw^2 + x^2w^2 + 2xw^2 + 2w^2 - 2xy^2w + 4xyw - 2x^3w - 4x^2w - 4xw + \\
x^2y^2 - 2x^2y + x^4 + 2x^3 - 7x^2 - 18x - 9 \leq 0 \wedge z - 1 \leq 0 \big] \vee [y-1 \leq 0 \wedge z - 1 \leq 0] \Big].
\end{gathered} \tag{6.13}$$

The output formula is not of great interest to solving the problem; the CAD constructed for (6.12) is needed for any substantial analysis. However, it is interesting to try and deconstruct (6.13). The first five terms state that the ladder should have both endpoints in the second quadrant of the plane, and that the ladder should have length 3. The remainder of (6.13) is a large disjunction of clauses describing the valid positions. The first clause of this disjunction describes the ladder being entirely within the vertical corridor, and the final clause describes the ladder being entirely in the horizontal corridor. The remaining three clauses characterise the intermediate positions. Analysis of the decompositions these equations describe requires knowledge of the adjacency of the CAD of $\mathbb{R}^4$: this is far from trivial and will be discussed in Section 6.3.6.

When constructing a CAD, and producing an equivalent formula, QEPCAD uses a host of techniques, including partial CAD techniques (Section 2.4.2) and equational constraints (Section 2.4.4) to simplify its calculations. We can suppress many of these by using the `full-cad` command, which greatly increases the difficulty of constructing a CAD. Constructing a `full-cad` of (6.12) takes just over a full day of computation (88238.442 seconds) and produces 1691473 cells. The formula QEPCAD produces in this case is almost identical to (6.13), although a couple of cases are split differently.

A useful technique to attempt to speed up the construction is to introduce quantifiers. In this case we can existentially quantify an endpoint of the ladder, which leads to a CAD

defining the valid positions of the opposite endpoint. Prefixing (6.12) with $(\exists\, w)(\exists\, z)$ will characterise the position of the (x, y) endpoint and takes QEPCAD just over 50 minutes (3052.753 seconds) to construct a CAD with 5453 cells. This sharp reduction will be due to the reduced dimension of the CAD produced ($\mathbb{R}^2$ rather than $\mathbb{R}^4$) and the use of partial CAD techniques, which can use these quantifiers to simplify the lifting stage. The quantifier-free formula that QEPCAD produces is

$$x \leq 0 \wedge y \geq 0 \wedge [x + 1 \geq 0 \vee y - 1 \leq 0], \tag{6.14}$$

which is clearly stating that the point is within the original corridor. This is to be expected as the quantified version of (6.12) is asking for those points where it is possible to place an end of the ladder and find a valid position to place the other endpoint. There is clearly a large redundancy in creating such a CAD however as the minimal CAD to describe the corridor contains only 17 cells.

This existential partial CAD is not enough to solve the path finding problem, and (6.14) contains little information. However, this is a useful experiment to test the feasibility and complexity of a CAD problem: the original formulation from [Dav86], given in (6.7), remains infeasible under the quantification $(\exists\, w)(\exists\, z)$. Note also, that if a quantified problem does not return the entire corridor then it can identify invalid regions where no placing of the ladder can occur. If these invalid regions separate the start and end positions into two distinct connected components, then it can be deduced that no valid path exists.

We can use the `p-2d-cad` command in QEPCAD to produce a visualisation of the two-dimensional CAD (the induced CAD of $\mathbb{R}^2$ if the CAD has dimension 3 or greater). Figure 6.6 shows the representation for the two-dimensional CAD for the existentially quantified version of 6.12 (without quantifiers a similar diagram is produced, but with the valid region simplified to omit all internal cell boundaries within the corridor). The horizontal axis shows x in the range $[-7, 2]$, and the vertical axis shows y in the range $[-2, 7]$. There is a step size of 0.0025, which means that if two stacks are within 0.0025, with respect to x, or two intra-stack cells are within 0.0025, with respect to y, then they will be indistinguishable on the diagram.

It is clear from Figure 6.6 how complicated this seemingly simple problem is. It is easy to identify important cell boundaries in the CAD that demonstrate edge cases of the Piano Mover's Problem: for example, when the ladder is stuck abutting the corner. However, there are clearly many boundaries with little or no significance to answering the question at hand. It would obviously be of great use to develop further CAD technology

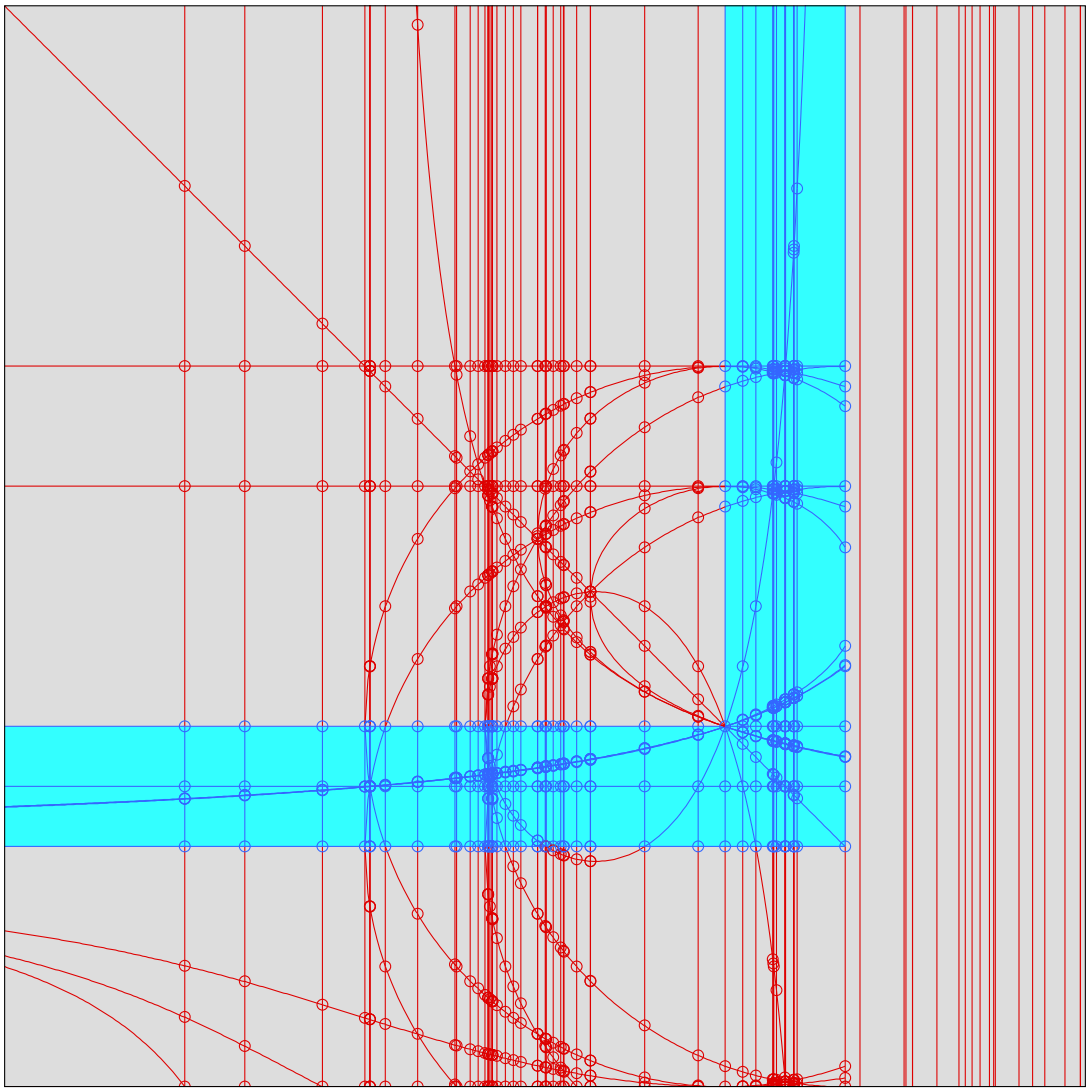


Figure 6.6: A two-dimensional CAD of the (x, y)-configuration space constructed for the piano mover's problem from (6.12).

that removes these spurious boundaries.

Remark 6.4.
MATHEMATICA can produce a cylindrical formula in 558.721 seconds, but for this application such a formula is not sufficient to deduce paths (since that will require knowledge of cell adjacencies and boundary cells, which cannot be inferred from the formula).

6.3.6 Adjacency for the Piano Mover's Problem

One reason for working in four-dimensional configuration space (as opposed to the real space that [Wan96, YZ06] consider) is that the constructed CAD can be used to construct a valid path, as well as determine the existence of such a path. To construct a path the adjacency and connectedness of the cells needs to be decided. Previous work on adjacency in CAD is discussed in Appendix A. The original approach of [ACM84b] for two dimensions was extended to three dimensions in [ACM88] but is not easily generalised further and often requires well-behaved input. Four-dimensional adjacency is currently not implemented within existing technology, and would be a hugely expensive and complicated computation. Possible improvements to adjacency algorithms which may be appropriate for the piano mover's problem will be discussed in Appendix A.

In [SS83b] the authors considered adjacencies between cells in the top two layers (of dimension n and $n-1$). For our expression of the problem we have an equational constraint so actually need the adjacencies between cells of dimension $(n-1)$ and $(n-2)$ so this theory does not apply.

6.3.7 Choosing a Formulation

Comparing (6.12) to (6.7) there are some indicators that our new formulation is more appropriate for CAD. In particular, the new formulation involves polynomials of lesser degree: quadratic polynomials instead of cubics.

We can use the `sotd` metric from Definition 2.42 (from [DSS04]) to measure this. Calculating the `sotd` of the input polynomials, which we denote `sotd*`, of the original formulation gives 100 whereas the new formulation has an `sotd*` of only 33.

As originally defined in [DSS04], the `sotd` should be computed for the entire projection set. Doing so still indicates the new formulation is better, but the total `sotd` drops only from 2006 to 1693. The size of these total `sotd` values emphasises the size of the projection sets produced, with over 100 univariate polynomials alone being produced in both formulations. It is therefore impractical to compute the `ndrr` from Definition 5.1

Formulation	Cell Count	`sotd*`	`sotd`	`ndrr`	`sowtd`
Davenport	—	100	2006	367	148
Davenport (∃)	—	100	2006	367	92
New Formulation	285419	33	1693	301	72
New Formulation (∃)	5453	33	1693	301	46
McCallum	16138	68	32	5	70
Wang	19	19	98	17	27
Yang-Zeng	5	35	39	2	23

Table 6.10: Heuristic values for various descriptions of the Piano Mover's Problem.

(from [BDEW13]) for the formulations directly. We can compute the `ndrr` for each univariate polynomial separately (which risks over counting by considering roots multiple times), which gives 367 for the original formulation and 301 for the new formulation.

We can consider the `sotd` (at the top level and full projection set) and `ndrr` for the alternative formulations of the piano mover's problem, which are summarised in Table 6.10. Note that the `sotd` for the McCallum formulation is actually lower for the full projection set than only at the top level due to repeated factors in the input.

None of the current heuristics incorporate quantifiers: their primary use is variable ordering where quantifiers are involved passively by restricting possible orderings. Quantifiers clearly have a huge effect on the feasibility of a formulation. We try to incorporate the effect of quantifiers along with variable ordering into the following heuristic, `sowtd`.

Definition 6.8.
Let a CAD problem be defined with respect to the ordered variables $x_1 \prec x_2 \prec \cdots \prec x_n$. For each variable x_i we assign a weight, $w(x_i)$: if x_i is unquantified then $w(x_i) = i$, and if x_i is quantified then $w(x_i) = i/2$. We define the **sum of weighted total degrees**, denoted `sowtd`, of a problem Φ (with polynomial set F) to be

$$\texttt{sowtd}(\Phi) = \sum_{f \in F} \sum_{m \in f} \sum_{i=1}^{n} w(x_i) \cdot \deg_{x_i}(m);$$

where m ranges over the monomials in f.

Table 6.10 also lists the `sowtd` values for each description of the Piano Mover's Problem. The `sowtd` values align with the cell counts for the formulations and seem a fair indication of the magnitude of each one. It would be of interest to investigate the behaviour of `sowtd` further: in particular to see if it be used to predict variable ordering

Length	EC-CAD Cells	EC-CAD Time (s)	∃ EC-CAD Cells	∃ EC-CAD Time (s)
3	285419	16286.431	5453	2941.024
2	314541	9863.950	5353	1922.837
5/4	404449	33042.101	5589	7312.347
3/4	446787	13146.195	4347	69.690
3 `full-cad`	1691473	88238.442	—	—

Table 6.11: CADs of (6.12) modified by varying ladder length. We compare both non-quantified and quantified versions (where the input formula was preceded by $(\exists w)(\exists z)$ as indicated by ∃ in the table).

or equational constraint designation.

6.3.8 Generalisations of the Problem

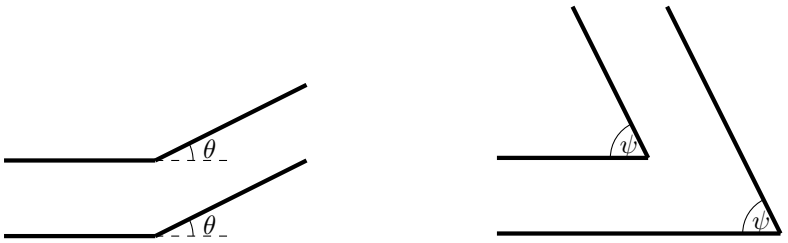
Different Lengths of Ladder

The original Piano Mover's Problem in [Dav86] and our description in (6.12) considers a ladder of length 3. We know, from simple geometric reasoning, that the maximal length of ladder sufficient to get through the corridor is $\sqrt{8}$. We can also deduce that any ladder of length $\sqrt{2}$ or less will be able to reverse orientation within the corridor.

We can adapt the new description of the Piano Mover's Problem in (6.12) to various lengths. We consider the following four representative examples that cover the four possible cases:

- **Length 3:** Ladder cannot traverse the corridor.
- **Length 2:** Ladder can traverse the corridor but is unable to reverse its orientation.
- **Length $\frac{5}{4}$:** Ladder can traverse the corridor and is able to reverse its orientation, but only within the 'corner'.
- **Length $\frac{3}{4}$:** Ladder can traverse the corridor and reverse its orientation at any point within the corridor.

Table 6.11 gives the cell counts and timings for all four lengths with and without existential quantifiers $(\exists\, w)(\exists\, z)$. It also gives the cell count and timing for the `full-cad` of the length 3 ladder as a comparison (there is little reason to compute a `full-cad` for all lengths as it would not be used in practice). As we have an explicit equational



(a) Generic obtuse angled corridor. (b) Generic acute angled corridor.

Figure 6.7: Angled corridors for the Piano Mover's Problem.

constraint (the equation defining the length of the ladder) QEPCAD can automatically apply the theory of equational constraints.

The results of Table 6.11 are not necessarily intuitive. In the un-quantified formulation the length 3 ladder produces the least cells, but the length 2 ladder is significantly quicker than all other lengths. When quantified, the lengths all produce similar numbers of cells, with length 3/4 producing the least cells and being substantially quicker than the other lengths (with length 5/4 substantially longer than the other lengths).

Angled Corridors

We can generalise the Piano Mover's Problem considered in [Dav86] to a non-right angled corridor. We can easily consider the two cases of an obtuse angled corridor (Figure 6.7a) and an acute angled corridor (Figure 6.7b).

We can easily convert the equations of the walls in Figures 6.7a and 6.7b into a formula describing the new set of invalid positions (given in detail in [WDEB13]). We proceed in the same manner as for the right-angled corridor (Section 6.3.4) by eliminating the parameter t, taking the negation of the output, and then conjuncting with the length of the ladder. This stage is straightforward, although produces around $170,000$ cells when θ is $\pi/4$, and $100,000$ cells when ψ is $\pi/4$.

We can then use this formula to attempt to construct a CAD of the configuration space. The two cases mentioned above (when θ or ψ is $\pi/4$) aborted after QEPCAD had computed 50000000 cells (the limit imposed by the initialisation parameter `+N50000000`). This increase in cells compared to (6.12) is due to the fact the corridor is no longer aligned with the coordinate axes.

Generalising the methods of [Wan96] and [YZ06] is not straightforward. Whilst Wang's idea can be applied to the obtuse case (giving a maximal length of approximately 6.68), it does not suffice for the acute case (giving the wrong answer of 1.84). With an

acute corridor of angle $\pi/4$, a ladder of length $\sqrt{5}$ can pass through, but has to reverse orientation in the corner in the process. This orientation would be accounted for in our formulation of configuration space, but is not encoded in the geometrical reasoning of real space. Using the approach of [McC97] for angled corridors should be possible, although care may need to be taken to ensure that certain trigonometric identities hold.

6.3.9 Constructing sub-CADs for the Piano Mover's Problem

In Chapter 4 the idea of a cylindrical algebraic sub-decomposition (sub-CAD) was introduced. Two particular types of sub-CAD were introduced: layered and variety sub-CADs. We consider their applications to the Piano Mover's Problem.

Lifting to a Layered Variety sub-CAD

All the cells that are valid in configuration space must lie on the three-dimensional variety described by $(x-w)^2 + (y-z)^2 = \ell^2$ (where ℓ is the length of the ladder). Therefore we can construct a variety sub-CAD with respect to this equational constraint to help tackle the Piano Mover's Problem.

On this manifold, the cells of greatest importance are those that are full-dimensional (with respect to the variety). We can therefore construct a 1-layered variety sub-CAD which will contain the 3-dimensional cells satisfying the length constraint. To tackle the problem we also require knowledge of the adjacency of these cells. We therefore need the cells on the variety of one less dimension (two-dimensional cells for this example): adjacencies of three-dimensional cells through one-dimensional or zero-dimensional correspond to infeasible situations in the real space (such as a robot having to "tightrope walk" an infinitesimally thin cell) and so are unnecessary. Therefore a 2-layered variety sub-CAD should be sufficient to answer the Piano Mover's Problem and provide a path.

We use the implementation of sub-CAD procedures in `ProjectionCAD` (discussed in Appendix C). We begin by constructing a 1-layered variety sub-CAD. Constructing the equational constraint projection set produces 11 polynomials (in $\mathbb{R}[y, w, z]$) and constructing a 1-layered sub-CAD of $\mathbb{R}^3$ takes 124.22 seconds in Maple to produce 64764 cells. Lifting over this sub-CAD to the variety takes a further 196.672 seconds, producing 101924 cells. This obviously offers substantial savings over computing a complete CAD with Qepcad in both cells and time.

It is not yet feasible to construct the 2-layered variety sub-CAD (or complete variety sub-CAD) within Maple. With the inclusion of partial CAD techniques or utilising the simple inequalities as discussed in Section 4.7.1 this should be feasible. Adjacency

computations are still an issue and are discussed further in Appendix A.

6.3.10 Conclusions on the Piano Mover's Problem

Although a generic symbolic solution to robot motion planning was provided in theory by [SS83b], it still remains infeasible to tackle even simple examples, such as the one considered in this section.

The simple example of moving a ladder through a right-angled corridor was shown in [Dav86] to be infeasible when tackled directly by the approach [SS83b]. This approach remains infeasible with current technology but by considering a different description of the proof it is possible to construct a CAD of the four-dimensional configuration space with QEPCAD. By considering the negation of the invalid positions a formulation was given with lower degree polynomials that was more suited for CAD.

It is possible to create a 1-layered variety sub-CAD with `ProjectionCAD` of the new description, although a 2-layered variety sub-CAD is still infeasible. The CAD alone does not provide a solution to the Piano Mover's Problem, and the adjacencies of the cells needs to be considered. This is beyond current technology, and it is an important question whether adjacency techniques could be adapted to consider cells on a variety.

An alternative approach is to use geometric reasoning to rephrase the problem, such as in [Wan96] and [YZ06]. This can be immensely powerful, reducing the problem to a relatively simple quantifier elimination problem. However, such an approach cannot provide a valid path, only reveal if such a path exists. Further, care needs to be taken when generalising their approaches, as demonstrated with angled corridors. It is also possible to adapt the configuration space, such as in [McC97] where the ladder was parametrised trignometrically.

This example demonstrates the importance of how a problem is described for CAD, and suggests that any major progress in tackling the robot motion planning problem symbolically may be just as likely from more appropriate formulations than from advances in technology or hardware. The new description of the Piano Mover's Problem also suggests some general strategies for expressing a problem. These are discussed in Section 6.4.

6.4 General Strategies for Describing a Problem for Cylindrical Algebraic Decomposition

The work of Brown in expressing the Joukowsky and Collision examples in Section 6.1 and the progress in the Piano Mover's Problem discussed in Section 6.3 indicate the benefit of an optimal expression of a problem for CAD. Further, the methods of generating and manipulating the descriptions of the problems were all straightforward and mathematically simple. Once an expression is given, then it may also be possible to precondition using Gröbner bases, as described in Section 6.2.

These examples suggest some general strategies for finding an optimal expression of a problem:

Consider Negation In both the Joukowsky example and the Piano Mover's Problem the negation of the problem was considered and proved more effective. In the Joukowsky example this was a logical negation of the formula whilst the Piano Mover's Problem was negated before constructing the formula (considering invalid positions).

Split into Sub-Problems In the example that Brown reformulated, he separates it into sub-problems that he can solve separately and combine the answers. The Joukowsky problem is fully quantified so each sub-problem returns a Boolean value which can be combined together easily. Even with one free variable (the Collision problem [Bro12]) combining the quantifier-free formulae is straightforward. If there is more than a single free variable then combining the output of sub-problems into a meaningful formula may prove difficult (and could involve another application of CAD).

Eliminate Parameters In the Piano Mover's Problem a sub-problem was generated by the presence of an extra parameter, t. An extreme version of the splitting into sub-problems mentioned above, we completely eliminate the parameter t before attempting to construct the CAD for the four free variables.

Maximising Chains of Conjunctions In general, it is a good idea to have chains of conjunctions which allow equational constraints (either of the whole formula or through TTICAD) to be utilised. This can influence other choices: input of the form $f \neq 0 \rightarrow \varphi$ should be negated to form $f = 0 \wedge \neg\varphi$.

Minimising Degree and Density One difference between the new expression of the Piano Mover's Problem and the one given in [Dav86] is the degree of the poly-

nomials involved. The new formulation involves quadratic polynomials that are relatively sparse in terms of degree 2 monomials (aside from the length formula, each polynomial has at most two quadratic monomials of the ten possible quadratic monomials). On the other hand, the original formulation contained four cubic polynomials, where almost every monomial has degree three. As the maximum degree of the polynomials in the problem features explicitly in the complexity estimates for CAD (Section 2.6) this is obviously an important consideration.

Gröbner Preconditioning As shown in Section 6.2, preconditioning may be beneficial if the problem involves a conjunction of equations (after which reduction of conjuncted inequalities and inequations can be used). To predict its effect the heuristic `TNoI` can be used.

Unfortunately there is no guaranteed algorithm for finding the best expression of a CAD problem. It is a necessarily bespoke process that requires a trial and error approach.

In [BG06] the manipulation of a mathematical expression for quantifier elimination is approached as an artificial intelligence problem. The authors develop a space of alternative formulations of an existentially quantified disjunctive normal form Boolean formula by substitution according to any linear equational constraints and grade each expression according to a set of criteria (that notes properties such as number of equalities/inequalities, number of conjunctions/disjunctions and number of existential/universal quantifiers). Mimicking search strategies such as A*-search, they find the formula with the smallest grade. This is an interesting systematic approach, which proves useful for the examples given. Pruning strategies are used to avoid an impractical search space, and care is taken to avoid explosion in formula size.

The heuristics investigated in Chapter 5, `TNoI` (Definition 6.7), and `sowtd` (Definition 6.8) can be used to help decide on particular choices. Incorporating these heuristics into a grading function that can then be used within the algorithm of [BG06] would seem an interesting and fruitful area of research.

6.5 Solotareff-3

6.5.1 Gröbner Preconditioning

We consider how Gröbner preconditioning can be used for the Solotareff-3 example discussed in Section 2.12:

$$(\exists\, u)(\exists v)\Big[[3v^2 - 2v - a = 0] \ \wedge\ [v^3 - v^2 - av - 2b + a - 2 = 0] \\ \wedge\ [3u^2 - 2u - a = 0] \ \wedge\ [u^3 - u^2 - au - a + 2 = 0] \ \wedge\ [1 \leq 4a] \ \wedge\ [4a \leq 7] \\ \wedge\ [-3 \leq 4b] \ \wedge\ [4b \leq 3] \ \wedge\ [-1 \leq v] \ \wedge\ [v \leq 0] \ \wedge\ [0 \leq u] \ \wedge\ [u \leq 1]\Big]. \quad (6.15)$$

Note that this has already been discussed within this chapter as it is sourced from the problems in [BH91].

We can see in (6.15) that the first four components are conjoined equational constraints, and so Gröbner preconditioning can be applied. As the inequalities are linear and univariate, there is little point investigating the effect of $\rightarrow_G^*$.

We need to compute separate bases for the two variable orderings. Both basis computations take around 0.025 seconds to compute, which is insignificant compared to the CAD construction time. The Gröbner bases for both $a \prec b \prec v \prec u$ and $b \prec a \prec v \prec u$ produce four polynomials, one of which is univariate (in a or b). We can therefore replace the four equational constraints with the appropriate basis and construct a CAD. The `TNoI` of the original four equational constraints is 9, and this is reduced to 8 and 7 for the two orderings, respectively. Therefore, `TNoI` predicts that for both orderings preconditioning should prove beneficial.

Tables 6.12 and 6.13 show the effect this preconditioning has. We can see that for $a \prec b \prec v \prec u$ preconditioning reduces the cell count by 48.3% for projection and lifting (with either Collins' or McCallum's projection operator) and the recursive regular chains algorithm. For $b \prec a \prec v \prec u$ we see a reduction in cell count of 93.4% for Collins' projection operator, and 93.1% for both McCallum's projection operator and the recursive regular chains algorithm. This aligns with the predictions by `TNoI` (and also that the second ordering showed a greater decrease in `TNoI`). It is also worth noting that following preconditioning all three CADs for the second order are now identical, which was not the case before preconditioning, and this fact should be investigated further.

Preconditioning is beneficial for QEPCAD in all four constructions and, interestingly, has a greater effect on the four-dimensional CAD (without $\exists$) than the `full-cad`, resulting in them changing ranking of efficiency. When using the incremental regular chains

Technique	Cells	Time	Section	Page
PL-CAD (Col)	54037	255.304	2.3	30
PL-CAD (McC)	54037	266.334	2.3	30
GB-CAD (Col)	28501	128.270	6.2.2	201
GB-CAD (McC)	28501	128.533	6.2.2	201
QEPCAD (full-cad no $\exists$)	54037	5.701	2.11	58
QEPCAD (no $\exists$)	1015	4.807	2.11	58
QEPCAD (full-cad)	349	4.782	2.11	58
QEPCAD	153	4.659	2.11	58
GB-QEPCAD (full-cad no $\exists$)	28501	5.198	6.2.2	201
GB-QEPCAD (no $\exists$)	73	4.669	6.2.2	201
GB-QEPCAD (full-cad)	625	4.628	6.2.2	201
GB-QEPCAD	63	4.801	6.2.2	201
RC-Rec-CAD	54037	327.421	2.5	43
RC-Inc-CAD	29	0.155	2.5.3	46
GB-RC-Rec-CAD	28501	219.280	6.2.2	201
GB-RC-Inc-CAD	29	0.148	6.2.8	220

Table 6.12: The Solotareff-3 problem with Gröbner preconditioning — variable order $a \prec b \prec v \prec u$.

algorithms there is no change after preconditioning. As discussed in Section 6.2.8 this is to be expected, as all equational constraints are utilised so there is no difference in the CAD whether using the original equations or a Gröbner basis.

6.5.2 Mathematical Reformulation

Whilst we have considered a particular formulation of the Solotareff-3 problem throughout this thesis, it is worth noting that there was a reformulation of the problem before any CADs were constructed.

In Section 2.12.1, the Solotareff-3 problem was stated, and a formulation derived from the definition of the uniform norm:

$$(\forall\, d)(\forall\, e)(\forall\, x)(\exists\, y)\Big[[-1 \leq x \leq 1] \rightarrow [-1 \leq y \leq 1] \wedge \\ [((x^4 + rx^3) - (ax + b))^2 \leq ((y^4 + ry^3) - (dy + e))^2]\Big]. \quad (6.16)$$

We note a few key features of this formulation: it is in seven variables, with three free variables; it contains six monomials with degree 8, and the key polynomial does not contain any monomials with degree less than quadratic; it contains no equational constraints; it contains a logical implication. These features suggest that this would be

Technique	Cells	Time	Section	Page
PL-CAD (Col)	161317	916.105	2.3	30
PL-CAD (McC)	154527	857.357	2.3	30
GB-CAD (Col)	10633	44.939	6.2.2	201
GB-CAD (McC)	10633	44.784	6.2.2	201
QEPCAD (full-cad no $\exists$)	154527	8.249	2.11	58
QEPCAD (no $\exists$)	2065	4.785	2.11	58
QEPCAD (full-cad)	1063	4.832	2.11	58
QEPCAD	375	4.687	6.2.2	201
GB-QEPCAD (full-cad no $\exists$)	11319	4.836	6.2.2	201
GB-QEPCAD (no $\exists$)	53	4.715	6.2.2	201
GB-QEPCAD (full-cad)	251	4.796	6.2.2	201
GB-QEPCAD	42	4.816	6.2.2	201
RC-Rec-CAD	154527	1154.146	2.5	43
RC-Inc-CAD	33	0.202	2.5.3	46
GB-RC-Rec-CAD	10633	113.710	6.2.2	201
GB-RC-Inc-CAD	33	0.161	6.2.8	220

Table 6.13: The Solotareff-3 problem with Gröbner preconditioning — variable order $b \prec a \prec v \prec u$.

a difficult problem for applying CAD, and indeed that is the case.

Following the reformulation of [Ach56], a theorem of Chebyshev was used to provide an alternative description of the problem. Restricting ourselves to the case when $r \geq 1$ (and specifying that in the formula) we get the following description:

$$(\exists\, u)(\exists\, v)\Big[[r \geq 1] \wedge [-1 < u < v < 1] \wedge [u^3 + ru^2 - au - 2b - 1 + r + a = 0] \wedge$$
$$[v^3 + rv^2 - av + 1 - r - a = 0] \wedge [3u^2 + 2ru - a = 0] \wedge [3v^2 + 2rv - a = 0]\Big]. \quad (6.17)$$

We compare the features of (6.17) with those of (6.16) mentioned above: it is now only in five variables, still with three free variables; there are four cubic monomials, six quadratic monomials, and the remaining are linear or constant; it contains four explicit equational constraints; it is a direct conjunction of terms. All of these features suggest that (6.17) is a better expression than (6.16), which is indeed the case.

For the example quoted in [BH91] that we have been considering in this thesis, we assign r to be -1 (appealing to symmetry) and make some bounds on a and b, which reduces (6.17) to (6.15). We can see that (6.15) has one fewer variable (which was free) and so a CAD of $\mathbb{R}^4$ evaluated down to $\mathbb{R}^2$ is needed. Furthermore, the degrees of certain monomials have been reduced (any new polynomials that have been added are simple

inequalities, so could potentially be used for sub-CADs, as described in Section 4.7.1) and the logical structure has been retained. As to be expected from the discussions in this chapter, this proves to be the most efficient expression and completes in a reasonable time.

6.6 Conclusion

In this chapter the issue of expressing a problem for CAD was investigated. Motivation was given in the form of two problems that were infeasible in their original format but proved relatively straightforward after some mathematical manipulation.

We conclusively showed that Gröbner preconditioning for CAD construction is a worthwhile area of study. Taking a Gröbner basis of a conjunction of equalities was shown to be generally beneficial, although there are cases where it can be detrimental to the complexity of the subsequent CAD. Experimental data was backed up by mathematical justification why this may be the case. A metric, `TNoI` (and its generalisation `TNoIF`), was given and it was shown to be well correlated to when preconditioning is beneficial, with mathematical reasons given for this behaviour. Further preconditioning was given by reducing inequalities with respect to the computed Gröbner basis. Experimentation suggests this is always beneficial (when it is possible) and complexity bounds on CAD support this.

An investigation into the "Piano Mover's Problem" of moving a ladder through a right angled corridor was also discussed. Whilst a simple problem for numerical techniques it was shown to be infeasible for CAD in [Dav86]. Whilst technology and CAD algorithms have both advanced significantly since then, this particular expression remains infeasible. A collection of successful work was described, but all required either non-trivial geometric reasoning or a trigonometric description of the problem (the former not allowing for the construction of valid paths, and the latter requiring non-trivial transformations). A new expression was given that was shown to be feasible, although still difficult. Generalisations for various ladder lengths and angled corridors were considered as well as the application of the sub-CAD theory from Chapter 4. All this work requires adjacency analysis, which is not possible with current algorithms.

These investigations led to some general strategies for expressing a problem for CAD. Unfortunately this is a rather bespoke process and nothing further than guidelines can be given, although the use of heuristics from Chapter 5 can prove useful.

Chapter 7

A General Framework for CAD

A range of new ideas and theory relating to CAD have been given in this thesis. These all interact with each other in a non-trivial manner. We now investigate their compositions and a general hierarchy of choices given as a guideline for how to tackle a problem.

CAD has applications outside of computer algebra, and so it is important to allow users to utilise advances in theory without a deep understanding of the underlying mathematics. We introduce the proof-of-concept software CADassistant, which demonstrates how tools can be used to let users appeal to a combination of heuristics and requirements for a problem to identify an appropriate statement for input into various CAD algorithms.

Author's Contribution and Publication

The work in this chapter is the author's. The experimentation and analysis are by the author, as is the implementation of CADassistant.

The discussion of TTICAD and Gröbner preconditioning in Section 7.1.2 was published in [BDEW13].

7.1 Interaction of Concepts

In this section we will discuss a variety of ways in which CAD concepts can interact. The work in this section is by the author, and has been partly published [BDEW13]. This survey is intended to indicate the complexity of using multiple CAD advances, and highlight that decisions are not independent. We will primarily be concerned with the projection and lifting based algorithms, as they offer the most formulation choices and applicable theories. As the work in this thesis has extended CAD technology, there are

few examples in the literature large enough to allow for investigating the interaction of these advances. Therefore the examples in this chapter have been created specifically for this thesis.

7.1.1 Interactions Previously Discussed

We briefly mention interactions that have already been discussed in this thesis, and summarise the findings.

Gröbner Preconditioning and Equational Constraints

In Section 6.2.8 the interaction between Gröbner bases and the theory of equational constraints was investigated. Preconditioning can be applied to any conjunction of equations in the formula. If the equations being consider for preconditioning are also equational constraints for the whole formula, then the equations in the basis produced can also be used to construct a CAD using equational constraint theory.

Experimentation in Section 6.2.8 confirmed that combining Gröbner preconditioning and equational constraints can very powerful: for the Solotareff-3 problem a sign-invariant CAD produces 154527 cells; with equational constraints alone it reduces to 48475; with preconditioning alone it reduces to 10633; and with both preconditioning and equational constraints it produces only 4809 cells (3.1% of the sign-invariant CAD).

There is an added complication when combining these techniques: building an equational constraint CAD with respect to most of the polynomials produced by the preconditioning fails (due to nullification on a cell of positive dimension). This is unsurprising as a purely lexicographical Gröbner basis provides a triangular structure, with polynomials in few variables of low levels. These polynomials will be automatically nullified due to the construction of the CAD. Therefore it seems prudent to always attempt to construct a preconditioned equational constraint CAD with a polynomial of the highest level first.

TTICAD and Layered/Variety sub-CADs

In Section 4.4.2 the construction of truth table invariant sub-CADs was discussed. The theory of layered sub-CADs, variety sub-CADs and their amalgamation transfer over to TTICADs. All three forms of sub-TTICAD have been implemented in the `ProjectionCAD` package as described in Section C.2. The layered sub-TTICAD algorithm computes the sub-decomposition directly rather than recursively. As the TTICAD algorithm be-

haves differently at the highest level, in both projection and lifting, it is not clear whether a recursive algorithm would be possible.

There is a slight limiting factor to the construction of variety sub-TTICADs. In the final lifting stage we must lift to the variety defined by the implicit equational constraint obtained by multiplying all the designated equational constraints from the subformulae. This is somewhat wasteful as we would really want to consider the variety for each separate formula and consider their union (for disjunctions) or intersection (for conjunctions). There is no immediate way to incorporate this into the lifting stage: there has been work [Str12] investigating the intersection and union of CAF cells so this is a possibility for future integration.

7.1.2 Gröbner Preconditioning for TTICAD

In Chapter 6 the preconditioning of an input to CAD by taking a Gröbner basis was investigated. In Chapter 3 the idea of a truth table invariant CAD was introduced and algorithms given for their construction by either projection and lifting or regular chains technology. This section will investigate the interaction of these concepts and discuss work by the author from [BDEW13].

We consider the application of Gröbner preconditioning to each subformula in a TTICAD problem. We know that preconditioning can be hugely beneficial, but occasionally detrimental, and it is of interest to see whether this effect amplifies when applied to each subformulae. This work extends the investigation of the interaction between Gröbner preconditioning and constructing a CAD with respect to an equational constraint.

For a TTICAD problem to be suitably complicated for Gröbner preconditioning requires subformulae to have multiple equational constraints. This complexity means there are few examples in the literature that are suitable and feasible for experimentation. We therefore do not give a full survey of results, but consider one example in detail.

Example 7.1.
Consider the following polynomials:

$$f_{1,1} := x^2 + y^2 - 1; \qquad f_{2,1} := (x-4)^2 + (y-1)^2 - 1;$$
$$f_{1,2} := x^3 + y^3 - 1; \qquad f_{2,2} := (x-4)^3 + (y-1)^3 - 1;$$
$$g_1 := xy - \frac{1}{4}; \qquad g_2 := (x-4)(y-1) - \frac{1}{4}.$$

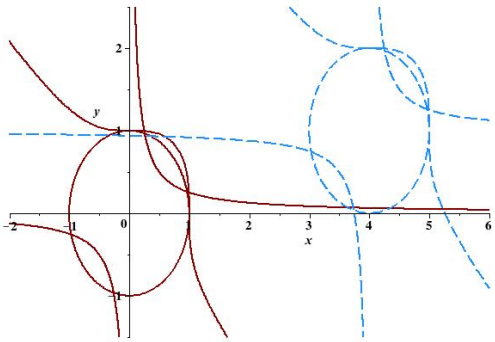


Figure 7.1: Plot of the polynomials in Example 7.1. The polynomials $f_{1,1}, f_{1,2}, g_1$ are shown in red (solid) and $f_{2,1}, f_{2,2}, g_2$ are shown in blue (dashed).

These are shown in Figure 7.1. We combine the polynomials into the formula Φ:

$$\Phi := \big[\,[f_{1,1} = 0 \wedge f_{1,2} = 0 \wedge g_1 > 0] \vee [f_{2,1} = 0 \wedge f_{2,2} = 0 \wedge g_2 > 0]\,\big].$$

We can construct a sign-invariant CAD of the polynomials in Φ with respect to the two variable orderings: $y \prec x$ and $x \prec y$. This gives CADs with 725 and 657 cells, as shown in Table 7.1.

To use TTICAD directly for Φ allows four possible formulations depending on equational constraint designation (as discussed in Section 5.2). Table 7.1 shows that all formulations of TTICAD offer a substantial saving in time and cell count. The values of `sotd` and `ndrr` on the entire projection set are also given and we can see that `ndrr` selects the optimal formulation (whilst `sotd` selects the worst ordering).

We can apply Gröbner preconditioning to both formulae in Φ separately, computing a Gröbner basis for $\{f_{i,1}, f_{i,2}\}$ with respect to a compatible purely lexicographical ordering. In both cases this computation is trivial and produces three polynomials in the basis. We denote the polynomials $\{\hat{f}_{i,1}, \hat{f}_{i,2}, \hat{f}_{i,3}\}$ listed in decreasing order of the leading monomials with respect to the order for the basis (although note that the polynomials will differ depending on the variable ordering).

We can see in Table 7.1 that applying Gröbner preconditioning can have a substantial effect on the complexity. The cell count can drop as low as 27 and 29 cells, taking under 0.1 seconds in both cases. As was demonstrated in Chapter 6, it is not always beneficial to precondition and there are multiple cases where a preconditioned formulation is less efficient than the worst TTICAD formulation (1 case for $y \prec x$ and 3 cases for $x \prec y$). It is testament to the power of TTICAD theory that even when preconditioning is harmful, it still performs much better than a sign-invariant CAD.

	CAD		TTICAD					GB+TTICAD				
	Cells	Time	Eq Const	Cells	Time	S	N	Eq Const	Cells	Time	S	N
$y \prec x$	**725**	**22.802**	$[1,1]$	153	0.818	**62**	12	$[1,1]$	**27**	**0.095**	**37**	**3**
			$[1,2]$	111	0.752	94	10	$[1,2]$	47	0.361	50	5
			$[2,1]$	121	**0.732**	85	9	$[1,3]$	93	0.257	50	9
			$[2,2]$	**75**	0.840	99	**7**	$[2,1]$	47	0.151	47	5
								$[2,2]$	83	0.329	63	7
								$[2,3]$	145	0.768	81	11
								$[3,1]$	95	0.263	46	10
								$[3,2]$	151	0.712	80	12
								$[3,3]$	209	0.980	62	16
$x \prec y$	**657**	**22.029**	$[1,1]$	125	0.676	**65**	14	$[1,1]$	**29**	**0.085**	**39**	**4**
			$[1,2]$	117	0.792	96	11	$[1,2]$	53	0.144	52	6
			$[2,1]$	117	0.728	88	11	$[1,3]$	97	0.307	53	7
			$[2,2]$	**85**	**0.650**	101	**8**	$[2,1]$	53	0.146	49	6
								$[2,2]$	93	0.332	65	8
								$[2,3]$	149	0.782	81	13
								$[3,1]$	97	0.248	48	11
								$[3,2]$	149	0.798	82	13
								$[3,3]$	165	1.061	65	18

Table 7.1: Various options of applying Gröbner preconditioning to Φ from Example 7.1 for use with TTICAD. For each formulation of Φ the designated equational constraints are given with the cell count, construction time (including time to construct Gröbner bases if appropriate), and values of `sotd` and `ndrr` on the projection set (denoted `S` and `N`).

It is obviously important to identify when it is beneficial to apply Gröbner preconditioning to a TTICAD problem. In this example `TNoI` (Definition 6.7) is of little use. In both orderings `TNoI` increases after preconditioning, which correctly identifies an increase in complexity if we compute a sign-invariant CAD. However, `TNoI` does not capture the TTICAD theory and so cannot distinguish between the different TTICAD formulations, nor predict it will be beneficial.

For Example 7.1 it appears that `ndrr` does well at predicting the optimal formulation both before and after preconditioning. Note that with only two variables, it is harder for `ndrr` to be deceived by higher dimensional geometry. Computing `sotd` for the TTICAD projection set correctly selects an optimal variable ordering after preconditioning, but performs poorly on the un-preconditioned formulations.

It is perhaps no coincidence that the optimal formulations following preconditioning designate the first equational constraint in each formula. The output of the `Groebner[Basis]` command in Maple orders the polynomials so that the first listed polynomial will be element of the basis with the largest leading monomial with respect to the order used to compute the basis (in this case the compatible purely lexicographical order). This identification and ordering is similar to the Brown heuristic and should be investigated

to see if it is a viable heuristic for preconditioning with TTICAD. Further, this heuristic could be applied to the general issue of equational constraint designation as discussed in Section 5.2.2.

Example 7.2.
In Section 6.2.8 it was shown that Gröbner preconditioning can also benefit the regular chains incremental algorithm for sign-invariant CAD but that often it has little effect as all equational constraints are utilised by the CAD algorithm. Following the work in Section 5.4 the improvement could also be due to a new input order of equational constraint as well as the preconditioning.

We can use the incremental TTICAD algorithm for Example 7.1. Before preconditioning it already produces a small number of cells: 29 cells when $y \prec x$ and 33 cells when $x \prec y$ (compared to an optimal 75 and 85 cells when using the projection and lifting algorithm). Preconditioning proves beneficial once again, reducing these down to 15 cells and 17 cells for the two variable orderings. This compares to an optimal 27 and 29 cells when using the projection and lifting algorithm with the preconditioned input.

Note that in the incremental algorithm there is no need for equational constraint designation and no chance for theoretical failure, unlike when projecting and lifting. This avoids the possibility of choosing a bad designation, such as $\hat{f}_{1,3}, \hat{f}_{2,3}$ in Table 7.1, which can increase the cell count and cancel out the benefit of preconditioning. The more sophisticated case analysis discussed in Section 3.5 allows for an even lower cell count than when using the projection-based TTICAD.

7.1.3 Gröbner Preconditioning and Layered/Variety sub-CADs

As with the interaction of Gröbner preconditioning with equational constraints, there should be little issue of incorporating preconditioning with the sub-CAD algorithms of Chapter 4. Constructing a preconditioned layered sub-CAD will be straightforward, with the two processes working independently. Constructing a preconditioned variety sub-CAD (or a preconditioned layered variety sub-CAD) will be possible, but likely only with respect to a few polynomials in the Gröbner basis. The triangular shape of a purely-lexicographic Gröbner basis ensures that only a small number of polynomials will contain the main variable x_n, and variety sub-CADs can currently only be constructed with respect to polynomials with main variable x_n (although it was described in Chapter 4 how the work could be extended).

Consider the Solotareff-B example again. A sign-invariant CAD using McCallum's operator produces 154527 cells, and we have seen that equational constraints and pre-

Technique	Cells	
PL-CAD	154527	—
EC-CAD	48475	31.4%
GB-CAD	10633	6.9%
GB-EC-CAD	4809	3.1%
GB-4-L-sub-CAD	10300	6.7%
GB-3-L-sub-CAD	8440	5.5%
GB-2-L-sub-CAD	4608	3.0%
GB-1-L-sub-CAD	1152	0.75%
GB-V-sub-CAD	1603	1.04%
GB-3-LV-sub-CAD	1385	0.90%
GB-2-LV-sub-CAD	904	0.59%
GB-1-LV-sub-CAD	272	0.18%

Table 7.2: Solotareff-B with a range of different CAD technologies.

conditioning can be applied separately or collaboratively to offer savings. Table 7.2 reproduces these results and considers constructing preconditioned sub-CADs. If we require a description of all regions satisfying the input formula, then we can use the preconditioned variety sub-CAD (the variety is with respect to the only element of the Gröbner basis that contains the main variable). This produces only 1603 cells, which is around 1% of the cell count for the sign-invariant CAD. We can also construct preconditioned layered variety sub-CADs that can reduce the cell count even further to 272 cells in the 1-layered case.

7.1.4 Gröbner Preconditioning, TTICAD, and sub-CADs

We can combine the concepts of Chapters 3, 4 and 6 to build preconditioned truth table invariant cylindrical algebraic sub-decompositions. We begin by looking at preconditioned variety sub-TTICADs and reconsider Example 7.1.

Example 7.3.
Recall Example 7.1, which involved constructing a TTICAD for:

$$\Phi := \big[\,[f_{1,1} = 0 \wedge f_{1,2} = 0 \wedge g_1 > 0] \vee [f_{2,1} = 0 \vee f_{2,2} = 0 \wedge g_2 > 0]\,\big].$$

It was shown that preconditioning can be highly beneficial (although also detrimental) compared to computing a normal TTICAD.

We investigate the benefit of computing a preconditioned variety sub-TTICAD. Table 7.3 gives the result of computing a TTICAD, variety sub-TTICAD, preconditioned

	CAD Cells	Eq Const	TTICAD Cells	V-TTICAD Cells	Eq Const	GB-TTICAD Cells	GB-V-TTICAD Cells
$y \prec x$	**725**	$[1,1]$	153	64	$[1,1]$	**27**	—
		$[1,2]$	111	45	$[1,2]$	47	—
		$[2,1]$	121	51	$[1,3]$	93	—
		$[2,2]$	**75**	**30**	$[2,1]$	47	—
					$[2,2]$	83	**26**
					$[2,3]$	145	56
					$[3,1]$	95	—
					$[3,2]$	151	60
					$[3,3]$	209	88
$x \prec y$	**657**	$[1,1]$	125	48	$[1,1]$	**29**	—
		$[1,2]$	117	47	$[1,2]$	53	—
		$[2,1]$	117	47	$[1,3]$	97	—
		$[2,2]$	**85**	**34**	$[2,1]$	53	—
					$[2,2]$	93	**46**
					$[2,3]$	149	62
					$[3,1]$	97	—
					$[3,2]$	149	62
					$[3,3]$	165	64

Table 7.3: Constructing a Gröbner preconditioned variety sub-TTICAD from Example 7.1.. For each formulation of Φ the designated equational constraints are given with the cell count, construction time (including time to construct Gröbner bases if appropriate), and values of `sotd` and `ndrr` on the projection set (denoted `S` and `N`).

TTICAD, and preconditioned variety sub-TTICAD.

We can note some interesting properties of Table 7.3. As it is simply a subset of cells, the variety TTICADs all have lower cell counts than the complete TTICADs. As discussed in Example 7.1, preconditioning for TTICAD is beneficial overall, but can be more costly depending on the designation of equational constraints. We note that the preconditioning is marginally more effective than lifting to the variety, although the difference is minimal and this is a relatively small example.

When constructing a preconditioned variety TTICAD we see that five of the nine possible designations result in an error. This is due to $\hat{f}_{1,1}$ and $\hat{f}_{2,1}$ not containing the relevant main variable for variety lifting. By necessity, the optimal designation for a preconditioned variety sub-TTICAD is therefore different from a preconditioned TTICAD. However, if we only designations without $\hat{f}_{1,1}$ or $\hat{f}_{2,1}$, the optimal orderings agree.

For variable ordering $y \prec x$ combining all three theories proves the most efficient, reducing 725 cells in a full sign-invariant CAD to 26 cells (3.6%). However, for $x \prec y$ combining all three theories is not the most efficient. A full sign-invariant CAD produces 657 cells and the optimal preconditioned variety sub-TTICAD produces 46 cells (7.0%). The optimal variety sub-TTICAD produces fewer cells (34 cells, 5.2%) and the optimal

preconditioned full TTICAD produces the minimal 29 cells (4.4%).

We now demonstrate that the addition of more subformulae or more variables can further complicate the interaction of these three concepts.

Example 7.4.
Consider the three clause version of Example 7.3 where we include a third formula in Φ:

$$[f_{3,1} = 0 \wedge f_{3,2} = 0 \wedge g_3 > 0],$$

where

$$f_{3,1} := (x+4)^2 + (y+1)^2 - 1; f_{3,2} := (x+4)^3 + (y+1)^3 - 1;$$
$$g_3 := (x+4)(y+1) - \frac{1}{4}.$$

Table 7.4 displays the results of combining preconditioning, TTICAD, and sub-CAD techniques.

We see that once again, each theory proves useful individually, with a preconditioned TTICAD again more powerful than a variety sub-TTICAD. However, we see that for both variable orderings the optimal preconditioned variety sub-TTICAD has more cells than the preconditioned TTICAD.

Example 7.5.
We now consider a three variable version of Example 7.3, and see the effect is also amplified. Consider the following polynomials:

$$\begin{array}{ll} f_{1,1} := x^2 + y^2 + z^2 - 1; & f_{2,1} := (x-4)^2 + (y-1)^2 + (z+2)^2 - 1; \\ f_{1,2} := x^3 + y^3 + z^3 - 1; & f_{2,2} := (x-4)^3 + (y-1)^3 + (z+2)^3 - 1; \\ g_1 := xyz - \frac{1}{4}; & g_2 := (x-4)(y-1)(z+2) - \frac{1}{4}. \end{array}$$

We can combine them to form Φ in the same manner as Example 7.3 and attempt to construct various forms of CAD (with respect to the variable ordering: $z \prec y \prec x$).

There are 2 equational constraints for each formula, giving 4 designations for TTICAD. Preconditioning produces Gröbner bases with 5 polynomials for each formula, resulting in 25 possible formulations for preconditioned TTICAD and variety sub-TTICAD. Therefore there are 55 possible formulations for the single variable ordering (making 330 formulations if the variable ordering is not fixed).

We consider every possible formulation for TTICAD, variety sub-TTICAD, preconditioned TTICAD, and preconditioned variety sub-TTICAD. The formulations shown

Variables	CAD	EC	TTI	V+TTI	GB+EC	GB+TTI	GB+V+TTI
$y \prec x$	**1789**	$[1,1,1]$	243	104	$[1,1,1]$	**39**	—
		$[1,1,2]$	231	101	$[1,1,2]$	63	—
		$[1,2,1]$	221	95	$[1,1,3]$	107	—
		$[1,2,2]$	189	82	$[1,2,1]$	63	—
		$[2,1,1]$	205	87	$[1,2,2]$	103	—
		$[2,1,2]$	189	82	$[1,2,3]$	159	—
		$[2,2,1]$	183	78	$[1,3,1]$	105	—
		$[2,2,2]$	**147**	**63**	$[1,3,2]$	153	—
					$[1,3,3]$	173	—
					$[2,1,1]$	63	—
					$[2,1,2]$	103	—
					$[2,1,3]$	167	—
					$[2,2,1]$	103	—
					$[2,2,2]$	159	**54**
					$[2,2,3]$	235	94
					$[2,3,1]$	161	—
					$[2,3,2]$	225	87
					$[2,3,3]$	265	108
					$[3,1,1]$	105	—
					$[3,1,2]$	161	—
					$[3,1,3]$	221	—
					$[3,2,1]$	161	—
					$[3,2,2]$	233	92
					$[3,2,3]$	305	130
					$[3,3,1]$	219	—
					$[3,3,2]$	299	125
					$[3,3,3]$	335	144
$x \prec y$	**1653**	$[1,1,1]$	187	72	$[1,1,1]$	**43**	—
		$[1,1,2]$	207	85	$[1,1,2]$	75	—
		$[1,2,1]$	207	85	$[1,1,3]$	111	—
		$[1,2,2]$	203	86	$[1,2,1]$	75	—
		$[2,1,1]$	207	85	$[1,2,2]$	123	—
		$[2,1,2]$	203	86	$[1,2,3]$	171	—
		$[2,2,1]$	203	86	$[1,3,1]$	111	—
		$[2,2,2]$	**175**	**75**	$[1,3,2]$	171	—
					$[1,3,3]$	179	—
					$[2,1,1]$	75	—
					$[2,1,2]$	123	—
					$[2,1,3]$	171	—
					$[2,2,1]$	123	—
					$[2,2,2]$	187	**66**
					$[2,2,3]$	247	98
					$[2,3,1]$	171	—
					$[2,3,2]$	247	98
					$[2,3,3]$	267	108
					$[3,1,1]$	111	—
					$[3,1,2]$	171	—
					$[3,1,3]$	179	—
					$[3,2,1]$	171	—
					$[3,2,2]$	247	98
					$[3,2,3]$	267	108
					$[3,3,1]$	179	—
					$[3,3,2]$	267	108
					$[3,3,3]$	247	96

Table 7.4: Constructing a Gröbner preconditioned variety sub-TTICAD from Example 7.4. For each formulation of Φ the designated equational constraints are given with the cell count.

TTICAD		V+TTICAD		GB+TTICAD		GB+V+TTICAD	
Designation	Cells	Designation	Cells	Designation	Cells	Designation	Cells
$[1,1]$	**359**	$[1,1]$	**108**	$[1,1]$	**37**	$[4,5]$	2125
				$[1,4]$	2543	$[5,5]$	**908**
				$[1,5]$	1097		
				$[2,1]$	1217		
				$[4,1]$	887		
				$[4,5]$	5473		
				$[5,1]$	1093		
				$[5,5]$	2463		

Table 7.5: Constructing a Gröbner preconditioned variety sub-TTICAD from Example 7.5. For each formulation of Φ the designated equational constraints are given with the cell count.

in Table 7.5 are the only ones not to time out or produce an error.

All formulations of preconditioned variety sub-TTICADs involving the first equational constraint in either clause resulted in theoretical failure (these equational constraints did not contain the main variable) and all other formulations timed out after 10 minutes.

We are in the unenviable position where using a pair of theories (either variety sub-TTICAD or preconditioned TTICAD) gives an efficient CAD, but using all three gives relatively poor results (indeed, worse than just computing a complete TTICAD) . This is because the optimal options for designation in preconditioned TTICAD involve the first polynomial in either basis, which do not contain the main variable (in this case, x). Note also that whilst preconditioning gives the optimal formulation across all options ($[1,1]$ with 37 cells), it also gives the worst formulation that does not time out ($[4,5]$ with 5473 cells).

This example was conducted with respect to a single variable ordering, and there is no guarantee that any of the above reasoning applies to the other 5 variable orderings. However, the symmetry in x, y and z suggests similar issues would occur.

Remark 7.1.
It might be that we can avoid certain failures due to sub-CAD techniques if the cell on which nullification occurs is omitted from the sub-CAD. Further, the regular chains TTICAD algorithm would prevent failure when constructing a preconditioned TTICAD (resulting in 21 and 25 cells for Example 7.4 and 43 cells for Example 7.5), but does not allow for the use of sub-CAD techniques.

In general, if each theory is beneficial then the combination is not necessarily more

efficient. Care must be taken particularly with Gröbner preconditioning which can have a negative influence (and the effect can vary in scale and between positive and negative depending on the other theories) whilst TTICAD and sub-CAD techniques are always beneficial individually.

In particular, the behaviour of the theories depend on the formulation of the problem, which will be discussed in the following section.

7.1.5 Interaction with Variable Ordering and Formulation

There is a further complication in that optimal choices for formulation can change depending on which variable order is used. We have seen this phenomenon at various points through this thesis and summarise in this section.

Variable Ordering and Gröbner Preconditioning

In Section 6.2 we assumed each problem for preconditioning had a fixed variable ordering. It is necessary to fix a variable ordering before preconditioning, as a Gröbner basis must be taken with respect to the compatible purely lexicographic monomial ordering. However, there are examples where the optimal ordering can change before and after preconditioning, as demonstrated in Example 7.6.

Example 7.6.
Consider the randomly generated polynomials:

$$f := -4x^2 + yz - z^2 - 5x - 2; \qquad g := 3y - 4z + 5;$$
$$h := x^2 - 3xz + y + 5z + 1.$$

Consider the formula Φ:

$$[f = 0 \wedge g = 0] \wedge h > 0.$$

We can apply Gröbner preconditioning in its simplest form by taking a Gröbner basis of f and g and taking its conjunction with $h > 0$. Table 7.6 gives the result of constructing a sign-invariant CAD before and after preconditioning for all 6 variable orders.

We can see that the optimal variable ordering for cell count changes from $z \prec x \prec y$ to $x \prec z \prec y$. Note that computing the `sotd`, `ndrr` or `TNoI` of the projection set after preconditioning all predict the optimal variable choice (but requires all six Gröbner bases to be computed along with their projections).

In this example all variable orderings benefit from preconditioning, as predicted by the fact that in all cases the `TNoI` of the input reduces from 8 to 7. However there

Ordering	CAD		GB+CAD	
	Cells	Time	Cells	Time
$x \prec y \prec z$	5183	28.758	641	2.595
$x \prec z \prec y$	1095	**5.186**	**203**	**0.852**
$y \prec x \prec z$	6865	43.287	1311	5.628
$y \prec z \prec x$	1831	12.415	1505	6.676
$z \prec x \prec y$	**1071**	5.417	361	1.119
$z \prec y \prec x$	1315	5.943	911	3.095

Table 7.6: Variable orderings before and after Gröbner preconditioning.

are two variable orderings where preconditioning is still not as efficient as some variable orderings without preconditioning. Given a ranking of all twelve options it is not a direct split into those preconditioned and not.

Variable Ordering and TTICAD

In Chapter 3 the idea of truth table invariance was introduced and in Chapter 5 the formulation choices of separating into subformulae and designating equational constraints were discussed. Example 7.1 demonstrates that optimal variable orderings can change with application of TTICAD: Table 7.1 shows that the optimal variable ordering for a sign-invariant CAD is $x \prec y$, whilst the optimal variable ordering for a TTICAD (whether preconditioned or not) is $y \prec x$.

Equational Constraint and TTICAD Designation and Variable Ordering

Interestingly, in Example 7.1 the choice of optimal equational constraint designation for TTICAD does not change with variable ordering. This is not always the case, as demonstrated in [BDEW13] where an example with two different variable orders has two different optimal equational constraint designations.

7.2 General Approach for Tackling a Problem with CAD

As shown in Examples 7.1, 7.2, 7.3, 7.4, 7.5 and 7.6, the interaction of all techniques and formulation choices is complicated. We now consider how we can deal with all formulations and theories simultaneously. In the following section we will discuss a general approach for tackling a problem by CAD.

7.2.1 Dealing with All Formulations and Theories

Before we can begin to formulate a problem for CAD we need to first express it in a manner that allows for CAD construction. This was discussed in Chapter 6 where the following general strategies were outlined:

- consider negating the formula;
- split into sub-problems if possible;
- eliminate parameters before constructing the final CAD;
- maximise chains of conjunctions;
- minimise degree and density.

As with the formulation choices from Chapter 5, it is possible to use heuristics to assist with these manipulations, but it is a much more bespoke process and cannot necessarily be conducted algorithmically (although hopefully the work of [BG06] could be adapted for this purpose).

We deal with producing this mathematical expression independently of the algorithm and formulation choices, to avoid adding further combinatorial complexity to the decision-making process. These two steps may not strictly be independent: it is possible, for example, that different expressions are optimal for different variable orderings, or that when considering different algorithms with well-orientedness conditions, various expressions are better suited. However, the expression of a problem can change the underlying (theoretically minimal) CAD and the formulation choices are more centred around the algorithmic construction, so it seems fair to separate the two.

Once we have a mathematical expression of a problem as a Tarski formula we may need to: select a variable ordering; choose a projection operator; designate equational constraints; decompose into subformulae; decide whether to apply preconditioning; decide which sub-CAD techniques to apply; and more. Considering all possible formulations and choices quickly becomes combinatorially overwhelming: a problem for TTICAD with three variables and two sub-formulae, each with two equational constraints, allows 990 formulations of [TTI]CADs and sub-[TTI]CADs (ignoring possible splitting of sub-formulae). Computing even basic heuristics for all of these formulations can easily negate any benefit of selecting an optimal formulation.

There is no predefined order in which these should be decided and the previous sections show that they are dependent on each other. We now try to describe a hierarchy of which to approach these decisions.

7.2.2 Hierarchy

The following is a suggested order for the choices:

1 **Mathematical Description:** Before we can start making any algorithm or formulation choices we need to have the mathematical expression of the problem. We can appeal to the suggestions from Chapter 6 along with heuristics to help with this decision, but there is not a general approach.

2 **Algorithm:** We know that constructing a CAD by projection and lifting or by regular chains behaves slightly differently. Although the underlying (theoretically minimal) CAD does not change, different algorithms can produce different sized CADs and formulation choices can be dependent on the algorithm used so it is important to select it immediately. In general it appears best to select the regular chains algorithm, if possible, but this has not been thoroughly investigated, and if sub-CADs or partial CADs are needed then projection and lifting is the only choice.

3 **Projection Operator (if applicable):** If constructing a CAD through projection and lifting, the choice of projection operator is straightforward. The projection operators of Collins, Collins–Hong, McCallum and Brown–McCallum are successive subsets:

$$\mathbf{C}\mathbf{P}(A) \supset \mathbf{CH}\mathbf{P}(A) \supset \mathbf{M}\mathbf{P}(A) \supset \mathbf{BM}\mathbf{P}(A).$$

Further, if an equational constraint exists, or the problem can be split into subformulae then the equational constraint operator, $\mathbf{M}\mathbf{P}_E(A)$, or TTICAD operator, $\mathbf{TTI}\mathbf{P}_{\mathcal{E}}(\mathcal{A})$, should be used. Depending on the formulation, certain projection operators may not be valid (due to well-orientedness conditions), but this will not be discovered until the lifting stage of construction. If this is the case, then the next best projection operator should be used.

4 **Variable Ordering:** We have repeatedly seen that variable ordering is key to the complexity of a problem. It is arguably the most important choice and further decisions will be dependent on variable ordering. It should therefore be selected before the other choices, and can be decided with heuristics (Brown, `sotd`, `ndrr`, layered) which can be selected with machine learning (Section 5.3).

5 **Formula Decomposition (if applicable):** If constructing a TTICAD then there may be a choice of formula decomposition. Although it is generally advantageous to separate into as few formulae as possible (maximising the effect of the equational

constraints), this is not always the case for projection and lifting TTICAD, and the decision method described in Section 5.2.3 can be used to make this decision.

6 **Gröbner Preconditioning (if applicable):** We need to have decided a variable ordering and separated into subformulae before potentially applying Gröbner preconditioning (as described in Chapter 6), and any preconditioning should be applied before designating any equational constraints or using a sub-CAD technique. Therefore, the decision regarding preconditioning should be made next, using `TNoI` (Definition 6.7) or some other measure.

7 **Constraint Designation (if applicable):** Next, the choice of equational constraint designation should be made if using a projection and lifting algorithm. If an incremental regular chains algorithm is being used then the order of input should be decided. These decisions can be made with a variety of heuristics as was discussed in Chapter 5.

8 **Sub-CAD Techniques (if applicable):** As constructing a sub-CAD (Chapter 4) will always produce a subset of the cells in a complete CAD, the decision can be made independently and after all other choices. If equational constraints are present (explicit or implicit) then a variety sub-CAD may be appropriate, and if only generic solutions or those of a certain dimension are needed then a layered sub-CAD may be appropriate.

This hierarchy is shown diagrammatically in Figure 7.2. Most of these decisions have the opportunity to influence each other so it may be necessary to work non-sequentially, returning to previous steps to alter them with respect to later decisions.

7.2.3 Identifying General Classes of CAD Problems

In [McC93] and [Str00] it was noted that if a CAD problem consists purely of strict inequalities then any cells that satisfy all conditions must necessarily be full-dimensional. Therefore a 1-layered sub-CAD is sufficient, and highly efficient, for this class of problems.

Similarly, if a problem consists purely of a conjunction of equalities, then Section 6.2.8 demonstrated that the incremental regular chains algorithm is the sensible choice. As it can utilise all equational constraints, it will effectively solve the problem and construct the minimal CAD around the solutions.

Extending the idea of [McC93, Str00] we could try to identify classes of problems for which a 1-layered variety sub-CAD will suffice. Given a problem of the form $f = 0 \wedge g > 0$

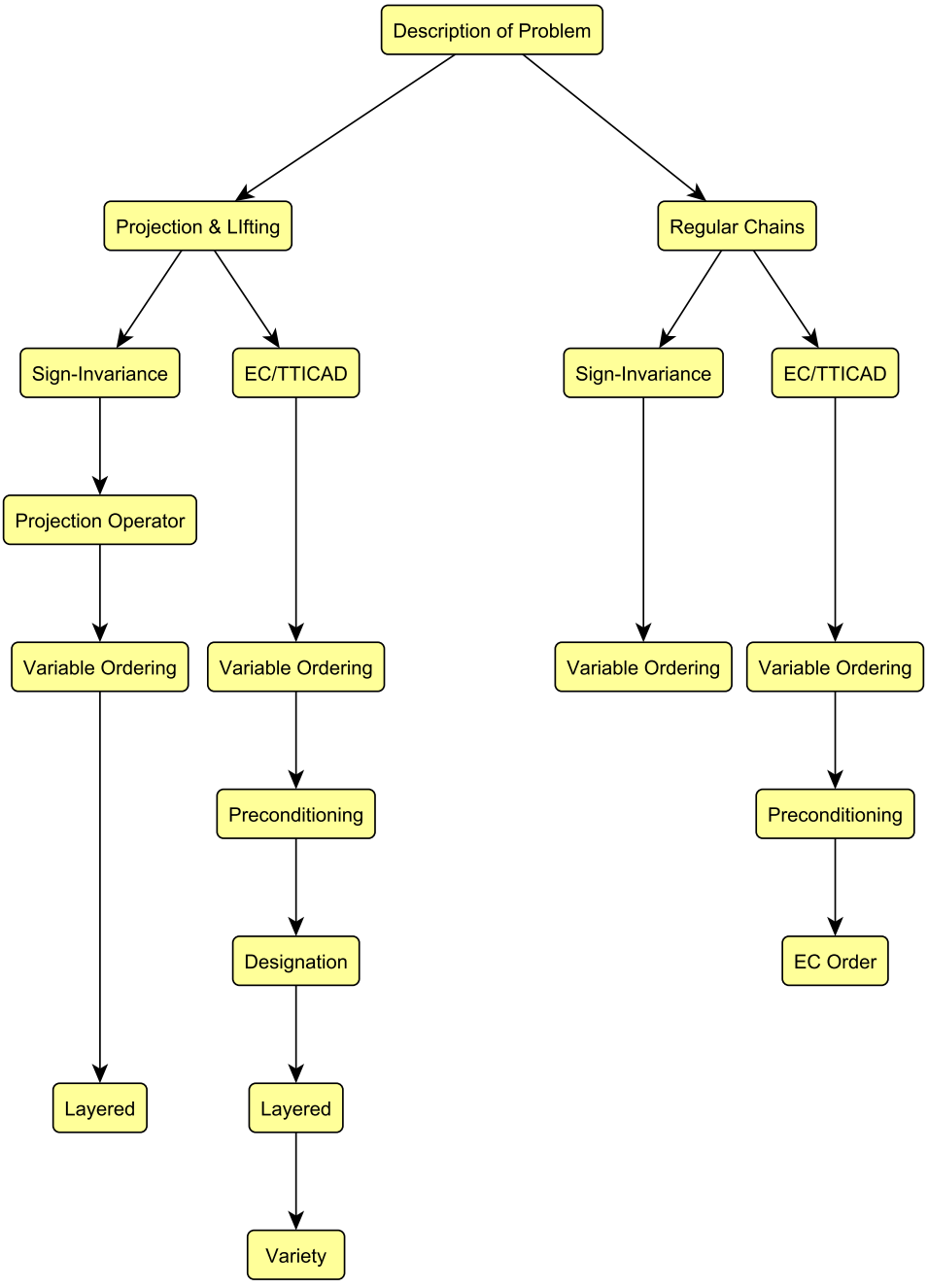


Figure 7.2: Decision hierarchy for a CAD problem.

where f defines a variety of co-dimension 1 then the full-dimensional cells on the variety will describe at least some of the solutions. In certain cases these cells will describe all the valid regions, and a condition to determine when this is the case would be highly valuable.

Ideally, we could identify a collection of classes to dictate when certain algorithms are well-suited or sufficient. This could be incorporated directly into CAD algorithms or into a separate piece of software, such as CADassistant described in Section 7.3. This is viewed as important future work, which would extend the applicability of the work in this thesis significantly.

7.3 Proof-of-Concept User Software — CADassistant

CADassistant is a proof-of-concept tool for enabling a user to take advantage of advances in CAD theory (including the ones described in this thesis) without knowledge of the underlying mathematics. It has only basic functionality and is intended to demonstrate the potential of such a tool.

The code is freely available[1] and is implemented in Python (further details of the implementation are given in Section C.4).

The user runs the tool from the command line and CADassistant can be run in interactive (the default) or manual modes:

```
> python CADassistant.py interactive
> python CADassistant.py manual
```

The user then gives details of the problem either directly (in `manual` mode) or through answering a sequence of questions regarding the needs of the application (in `interactive` mode).

The decisions made in `interactive` mode centre around trying to find if there is an optimal way to solve the given problem. It can help identify if a layered sub-CAD or variety sub-CAD may be appropriate, if Gröbner preconditioning is possible, whether quantifier elimination is needed, and so forth.

The output is then given for the appropriate platform. Currently support is only given for Maple and Qepcad but other technologies (such as Mathematica, SyNRAC and Redlog) could be integrated in the future.

The implementation of CADassistant in Python is described in Section C.4. The problems are stored in an object from a hierarchy of classes: `CadProblem` for a ba-

[1]The code can be downloaded from `http://www.github.com/DavidJohnWilson/CADassistant`.

sic problem, `CadProblemMethod` if the method is also specified, and `CadTTICAD` if it is separated into separate formulae for TTICAD.

7.3.1 Sample CADassistant Session

We describe a sample CADassistant session to demonstrate its usage. On running the program in either interactive or manual mode the following is displayed, requiring input from the user. We will assume the following input for this session:

```
############################################################
#     CADassistant                                         #
#          by David Wilson (D.J.Wilson@bath.ac.uk)         #
#                                                          #
#     A tool for computing CADs with various technologies  #
#   and techniques.                                        #
#                                                          #
############################################################

Please enter a name for the CAD problem (or 'help'):
                        Sample CADassistant Problem
Please enter the polynomials for your problem,
 within square brackets and separated by commas:
                        [3*x^2+4*y-3, x^2-y^3,x^3-y^2,y-x]
Please enter the variables for your problem,
 within square brackets and separated by commas:
                        [x,y]
```

Manual Mode

Manual mode is intended for use by users who already have some knowledge of CAD or an implementation of CAD. It asks the following three questions to ascertain the kind of CAD required:

```
Please specify a construction method (default:
 projection&lifting):
                        projection
Please specify an invariance to build the CAD with respect to
 (default: sign-invariance):
                        truth table
Please specify any subCAD techniques to use (default: none):
                        variety
```

If the invariance condition is given as truth table invariance, then the decomposition into sub-formulae and equational constraint designation needs to be specified. This is done with respect to the order the polynomials were entered and the formulae are defined by a list of lists.

```
Polynomials are:
Poly 0: 3*x^2+4*y-3
Poly 1: x^2-y^3
Poly 2: x^3-y^2
Poly 3: y-x
Please enter in the clauses of the TTICAD (as a list of lists
 identifying the correct polynomials), or if dealing with
 equational constraints leave empty:
                        [[0,3],[1,2]]
```

For every subformula specified, the designated equational constraint needs to be specified. If no equational constraint is present in a particular clause then an empty answer can also be given.

```
Clause 0:
Poly 0: 3*x^2+4*y-3
Poly 3: y-x
Select the equational constraint for this clause:
                        3
Clause 1:
Poly 1: x^2-y^3
Poly 2: x^3-y^2
Select the equational constraint for this clause:
                        1
```

A summary of the problem is given, including the kind of CAD (using the acronyms in Appendix D) and TTICAD details (if appropriate).

```
Summary of TTICAD Problem:
    Name :  Sample CADassistant Problem
    Polys:  3*x^2+4*y-3, x^2-y^3, x^3-y^2, y-x
    Vars :  x,y
    CAD :   V-PL-TTICAD
    Clauses:    [0,3]   [1,2]
    EqCons :    [3]     [1]
```

The user is then asked if they wish to have the MAPLE code to construct the defined CAD:

```
Would you like the input for Maple?
                          yes
Cad := VTTICAD([[y-x,[3*x^2+4*y-3]],[x^2-y^3,[x^3-y^2]]],[x, y]);
```

The user can then use this command within MAPLE using the `ProjectionCAD` package to produce a sub-CAD with 18 cells.

Interactive Mode

In `interactive` mode less understanding of CAD is assumed of the user. As shown in the general hierarchy in Section 7.1, it is generally a good idea to select a variable ordering of the problem straight away.

The user is first asked if they wish to use a heuristic to select the variable ordering, or enter a predetermined order. On selecting to use a heuristic they have the option to select one manually or automatically from: Brown's heuristic `[B]`, `sotd [S]`, `ndrr [N]`, or the layered heuristic `[LAY]`.

If the user asks to select the heuristic automatically, they are given the choice to select a quick heuristic (where Brown's heuristic is used) or the most accurate (where the layered heuristic is used). Finally, the user is given code to run the heuristic in MAPLE with `ProjectionCAD` to then set the variable ordering.

```
Do you wish to use a heuristic to choose a variable ordering? [Y/n] :
                          Y
Please load Projection CAD to use any of the following heuristics.

Do you wish to pick the heuristic manually [M], or
 automatically [A]? [m/A] :
                          A
Do you want a quick heuristic that may be less accurate [Q], or a
 slower heuristic that is more accurate [S]? [Q/s] :
                          Q
Please copy the following code into your Maple window:
S:=VariableOrderingHeuristic([x, y], [3*x^2+4*y-3, x^2-y^3,
    x^3-y^2, y-x],heuristic='BrownBasic',SeeAll=false);
Please paste the output from the above command:
                          [x,y]
Variable ordering has been successfully changed.
```

The user is then asked if the problem contains just strict inequalities, in which case they are able to select whether to use the `LCAD` command in `ProjectionCAD` or the

`measure-zero-error` option in QEPCAD. The appropriate code is then given to the user for their chosen technology.

```
Does your problem involve only strict inequalities? [y/N] :
                          Y
You should use a 1-layered CAD.
Would you like to use ProjectionCAD [P] or Qepcad [Q]? [P/q] :
                          P
Please load Projection CAD and use the following input:
C:=LCAD( [3*x^2+4*y-3, x^2-y^3, x^3-y^2, y-x], 1,
    [x, y],method='McCallum'):
```

There is also basic functionality for Gröbner basis preconditioning. At the moment it is restricted to preconditioning the entire input (assuming a conjunction of equalities). If preconditioning is possible the user can use TNoI to predict if preconditioning will be beneficial, and is given code to compute the basis (and replace the polynomials for the given problem).

```
Does your problem involve just a conjunction of equalities that
 you can use Grobner preconditioning for? [y/N] :
                          Y
Do you wish to use TNoI to predict whether preconditioning
 will be useful? [Y/n] :
                          Y
Please run the following two lines of code:
TNoI:=proc(F): add(nops(indets(f)),f in F): end proc:
TNoIdiff := TNoI([3*x^2+4*y-3, x^2-y^3, x^3-y^2, y-x]) -
 TNoI(Groebner[Basis]([3*x^2+4*y-3, x^2-y^3, x^3-y^2, y-x],
  plex(op([x, y]))));
Is the value positive? [y/n] :
                          Y
Please copy the following code into Maple to compute the Grobner basis:
Groebner[Basis]([3*x^2+4*y-3, x^2-y^3, x^3-y^2, y-x], plex(op([x, y])));
Please copy the output:
                          [1]
```

In this case there are no solutions to the system of equations and so the basis is trivial, and the difference in `TNoI` is 8 (and therefore positive).

The user can then select different CAD algorithms in a similar way to the `manual` method.

7.3.2 Extending CADassistant

As discussed above, CADassistant is currently a proof-of-concept tool and the previous section only demonstrates basic functionality. There are obvious ways for the features of CADassistant to be extended. In particular: a wider range of CAD methods could be introduced; more subtle options for Gröbner preconditioning and the like; integration with the machine learning techniques used in Section 5.3; direct interface with Maple and Qepcad (avoiding the need for the user to copy and paste input and output).

7.4 Solotareff-3

We consider again the Solotareff-3 problem from [BH91]:

$$(\exists\, u)(\exists v)\Big[[3v^2 - 2v - a = 0] \;\wedge\; [v^3 - v^2 - av - 2b + a - 2 = 0] \\ \wedge\; [3u^2 - 2u - a = 0] \;\wedge\; [u^3 - u^2 - au - a + 2 = 0] \;\wedge\; [1 \leq 4a] \;\wedge\; [4a \leq 7] \\ \wedge\; [-3 \leq 4b] \;\wedge\; [4b \leq 3] \;\wedge\; [-1 \leq v] \;\wedge\; [v \leq 0] \;\wedge\; [0 \leq u] \;\wedge\; [u \leq 1]\Big]. \quad (7.1)$$

We consider how this problem fits within the general framework of CAD, and how the various choices affect its solution. Tables 7.7 and 7.8 show the results, for the two variable orderings, for all CADs and sub-CADs that are sufficient to solve the problem.

We can see that when using projection and lifting algorithms, all the relevant technologies complement each other to increase efficiency. For $a \prec b \prec v \prec u$ utilising equational constraints, through an equational constraint CAD or variety sub-CAD, proves more efficient than Gröbner preconditioning, whilst for $b \prec a \prec v \prec u$ the preconditioning is more powerful (even than a variety sub-CAD). Indeed, a preconditioned variety sub-CAD with the second ordering is the smallest projection and lifting CAD that can be constructed using the theory presented in this thesis.

When combining preconditioning with the equational constraint CAD or variety sub-CAD we see that the optimal variable order changes, with $b \prec a \prec v \prec u$ becoming 61.6% more efficient compared to the other variable ordering, whilst it was 66.6% less efficient for a sign-invariant CAD.

With Qepcad we have little control over the interactions and can only externally affect it through Gröbner preconditioning. It is interesting to note that the preconditioning has a greater effect when we omit quantifiers (constructing a CAD of $\mathbb{R}^4$ rather than $\mathbb{R}^2$) than specifying a `full-cad` (preventing the use of certain partial-CAD techniques and equational constraints). Without knowledge of the implementation of Qepcad it would

Technique	Cells	Time	Section	Page
PL-CAD (Col)	54037	255.304	2.3	30
PL-CAD (McC)	54037	266.334	2.3	30
EC-CAD (f_3)	20593	65.856	2.4.4	40
EC-CAD (f_4)	22109	102.781	2.4.4	40
V-CAD (f_3)	8195	63.387	4.2	114
V-CAD (f_4)	8953	95.233	4.2	114
GB-CAD (Col)	28501	128.270	6.2.2	201
GB-CAD (McC)	28501	128.533	6.2.2	201
GB-EC-CAD (g_4)	12513	55.749	7.1	249
GB-V-CAD (g_4)	4171	53.251	7.1	249
QEPCAD (full-cad no $\exists$)	54037	5.701	2.11	58
QEPCAD (no $\exists$)	1015	4.807	2.11	58
QEPCAD (full-cad)	349	4.782	2.11	58
QEPCAD	153	4.659	2.11	58
GB-QEPCAD (full-cad no $\exists$)	28501	5.198	6.2.2	201
GB-QEPCAD (no $\exists$)	73	4.669	6.2.2	201
GB-QEPCAD (full-cad)	625	**4.628**	6.2.2	201
GB-QEPCAD	**63**	4.801	6.2.2	201
RC-Rec-CAD	54037	327.421	2.5	43
RC-Inc-CAD	29	0.155	2.5.3	46
GB-RC-Rec-CAD	28501	219.280	6.2.2	201
GB-RC-Inc-CAD	29	0.148	6.2.8	220

Table 7.7: The Solotareff-3 problem with the general framework of CAD — variable order $a \prec b \prec v \prec u$.

be remiss to speculate why this may be the case, but it warrants further investigation.

When considering the regular chains algorithms, we have even fewer options for interaction: the recursive algorithm can only construct sign-invariant CADs and neither it nor the incremental algorithm have been adapted to admit sub-CADs. The recursive algorithm can only utilise preconditioning, which proves beneficial in both variable orderings (as it did for the projection and lifting algorithms). The incremental algorithm automatically utilises all four equational constraints in (7.1) and so explicitly requiring an equational constraint CAD has no effect. Similarly, preconditioning has no effect (as discussed in Section 6.2.8) and does not change the optimal variable ordering like when using projection and lifting algorithms.

Technique	Cells	Time	Section	Page
PL-CAD (Col)	161317	916.105	2.3	30
PL-CAD (McC)	154527	857.357	2.3	30
EC-CAD (f_3)	48475	175.139	2.4.4	40
EC-CAD (f_4)	63583	324.663	2.4.4	40
V-CAD (f_3)	19127	173.083	4.2	114
V-CAD (f_4)	25563	295.556	4.2	114
GB-CAD (Col)	10633	44.939	6.2.2	201
GB-CAD (McC)	10633	44.784	6.2.2	201
GB-EC-CAD (g_4)	4809	20.420	7.1	249
GB-V-CAD (g_4)	1603	20.053	7.1	249
QEPCAD (full-cad no $\exists$)	154527	8.249	2.11	58
QEPCAD (no $\exists$)	2065	4.785	2.11	58
QEPCAD (full-cad)	1063	4.832	2.11	58
QEPCAD	375	4.687	6.2.2	201
GB-QEPCAD (full-cad no $\exists$)	11319	4.836	6.2.2	201
GB-QEPCAD (no $\exists$)	53	4.715	6.2.2	201
GB-QEPCAD (full-cad)	251	4.796	6.2.2	201
GB-QEPCAD	42	4.816	6.2.2	201
RC-Rec-CAD	154527	1154.146	2.5	43
RC-Inc-CAD	33	0.202	2.5.3	46
GB-RC-Rec-CAD	10633	113.710	6.2.2	201
GB-RC-Inc-CAD	33	0.161	6.2.8	220

Table 7.8: The Solotareff-3 problem with the general framework of CAD — variable order $b \prec a \prec v \prec u$.

7.5 Conclusion

Whilst each advance described in this thesis is beneficial individually, we have shown that combining them is not straightforward. Certain combinations naturally work well together but when certain conditions are needed, such as well-orientedness, the only possible formulations may prove to be less efficient than using only a selection of advances. This was demonstrated through a collection of examples.

Unfortunately there is not a general algorithm to select an optimal combination of formulations and theories, but a hierarchy was given as a guideline for these choices. As the process is non-sequential, with later choices affecting earlier ones, care must be taken.

CADassistant, a proof-of-concept tool designed to help a user use CAD to solve a given problem was described. CADassistant is meant to demonstrate that whilst the interaction of the ideas in this thesis is complex, a computer can be used to assist

someone wishing to take advantage of them.

Chapter 8

Future Work and Conclusions

Whilst constructing a CAD can seem excessive for many applications, the use of various advances in CAD theory can tailor the output to the desired purpose and needs of a problem. It is important not only to devise new methods of constructing CADs, but also to understand the interaction of various improvements with each other.

We discuss how the work in this thesis can be extended in multiple directions and summarise the effect of the advances on the guiding example, Solotareff-3. Finally, the contributions of this thesis are summarised.

8.1 Future Work

Throughout this thesis we have noted possible extensions of the work and ideas for future investigation. We summarise these suggestions here:

- **Chapter 3: Truth Table Invariant CAD.**

    1. Identify conditions for when lifting with respect to the ResCAD set (Definition 3.7) will produce a TTICAD. This will allow for easy use in other projection and lifting CAD implementations.
    2. Extend the semi-restricted equational constraint projection operator to TTICAD. By using ${}_{\mathbf{TTI}}\mathbf{P}_{\mathcal{E}}(\mathcal{A}) \cup \{\text{disc}_{x_n}(g) \mid g \in \bigcup_{i=1}^{m} A_i \setminus E_i\}$ it may be possible to extend the TTICAD projection past the first projection level.
    3. Extend the TTICAD projection operator to include the work on bi-equational constraints when sub-formulae have multiple equational constraints.
    4. Compare the output of the projection and lifting TTICAD algorithm (which requires well-oriented input) and the regular chains TTICAD algorithm. This

can be used to help decide if the restriction of well-orientedness can be avoided.

5. Combine TTICAD with partial CAD techniques. This will likely require keeping track of sources of cells to simplify lifting with respect to each sub-formula.

- **Chapter 4: Cylindrical Algebraic sub-Decompositions.**

1. Identify classes of problems that different sub-CADs are well-suited for, to extend their application.
2. Implement and extend the idea of utilising simple inequalities in both the projection and lifting stages.
3. Consider how the regular chains algorithms could be adapted to incorporate the idea of various sub-CADs. It should be possible to restrict the complex cylindrical tree and decomposition, at least partially, according to dimension or a variety (but possibly only with respect to complex space).

- **Chapter 5: Formulation of Problems.**

1. Adapt Brown's heuristic, which is very effective for variable ordering, to other formulation issues such as equational constraint designation.
2. Investigate selecting a variable ordering with machine learning for different classes of problems (with more variables and different quantifier structures).
3. Investigate the application of alternative machine learning techniques to the problem of selecting a variable ordering.
4. Apply machine learning to other formulations issues.
5. Improve the efficiency of the layered heuristic by implementing a parallel version and incorporating other sub-CAD techniques.

- **Chapter 6: Mathematical Description.**

1. Investigate whether pseudo-remainder reduction with respect to Gröbner bases can offer greater savings.
2. Investigate how preconditioning affects the proportion of time spent in various parts of CAD algorithms: the projection against the lifting phase, or the complex decomposition against the `MakeSemiAlgebraic` phase.

3. Use machine learning to predict whether Gröbner preconditioning will be beneficial or not. This can be done either by selecting a heuristic or using the heuristics as features to decide directly.
4. Extend the work on the piano mover's problem to consider more difficult problems and to incorporate adjacency.
5. Investigate `sowtd`, which proved useful for the piano mover's problem, as a general heuristic.
6. Incorporate various heuristics into a grading function for use with the artificial intelligence algorithm of [BG06] to identify optimal mathematical expressions.

- **Chapter 7: General Framework.**

1. Investigate further the multiple interactions that exist between the different extensions to CAD.
2. Look at whether it is possible to extend variety sub-TTICADs by taking intersections of the variety sub-CADs for each sub-formula, rather than lifting with respect to the implicit equational constraint.
3. Investigate designating an equational constraint after Gröbner preconditioning and whether the lexicographic ordering the polynomials are presented in can be utilised.
4. Develop CADassistant to offer more options and more sophisticated decision techniques.

- **Other Extensions and Ideas:**

1. Investigate adjacency within CAD, as discussed in Appendix A. In particular:
   (a) Adapt and develop algorithms to consider adjacency in TTICADs and sub-CADs.
   (b) Develop the new idea of ℓ-dimensional path connectedness (Definition A.9), linking the topology and geometry of the problem with layered sub-CADs.
   (c) Investigate the new idea of an algorithmically minimal CAD (Definition A.6) to improve current algorithms.
2. Semi-monotonicity of sets [BGV13] generalises the idea of convexity to only require convexity aligned with axes (the direction of projection for CAD). Investigate whether such an idea could be used to construct a stronger CAD

where cells are cylindrical in multiple projection directions at once. Such a CAD would be more complex but could offer theoretical benefits: semi-monotone sets are topologically regular cells [BGV13].

3. Investigate he idea of order invariance, which is used in the proofs of the validity of certain projection operators. It is not clear if the regular chains algorithms generate order-invariant CADs, what the complexity cost of order-invariance is, and whether order-invariance guarantees CADs with particularly nice properties.
4. Extend previous work on parallelism in CAD [McC97, MD11] both by separating the problem (such as described in Section 6.1) and through the algorithm itself. A parallel implementation of the main CAD algorithm in `ProjectionCAD` (using the `Threads` package of Maple) would allow for greater investigation. There has also been recent work on utilising GPUs for real root isolation [TM12] which may prove useful to CAD construction.
5. Whilst most of the work on CAD has been done to minimise the number of cells produced, it may be worth investigating if this is always the desired output. An example given in [BD07] produces 3 cells with one variable ordering and doubly-exponential cells for all other orderings. The three cell description hides much of the behaviour of the function that may be necessary for applications and identifying such restrictions on variable orderings (outside of quantifier elimination) could prove important.

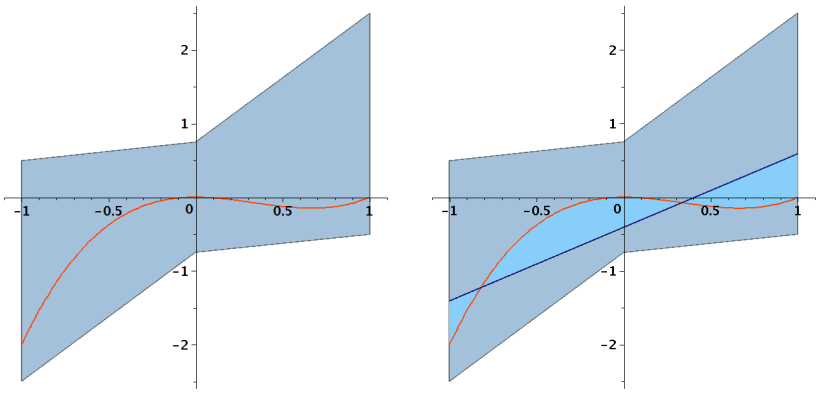
Most importantly, all the work in this thesis should be considered in relation to other CAD technology, such as Qepcad or Mathematica. This may be done directly, or by identifying alternative methods of constructing concepts introduced in this thesis.

8.2 Solotareff-3

We have been considering the Solotareff example as given in [BH91]:

$$(\exists\, u)(\exists v)\Big[[3v^2-2v-a=0]\ \wedge\ [v^3-v^2-av-2b+a-2=0]$$
$$\wedge\ [3u^2-2u-a=0]\ \wedge\ [u^3-u^2-au-a+2=0]\ \wedge\ [1\leq 4a]\ \wedge\ [4a\leq 7]$$
$$\wedge\ [-3\leq 4b]\ \wedge\ [4b\leq 3]\ \wedge\ [-1\leq v]\ \wedge\ [v\leq 0]\ \wedge\ [0\leq u]\ \wedge\ [u\leq 1]\Big]. \quad (8.1)$$

We have seen that Qepcad can be used to eliminate the variables in (8.1) and so



(a) Solotareff-3 problem. (b) Solution to Solotareff-3.

Figure 8.1: Solution to the Solotareff problem in three variables when $r = -1$.

solve the Solotareff problem in this case. Using the ordering $a \prec b \prec v \prec u$ we get the following equivalent quantifier-free formula:

$$a - 1 = 0 \wedge 4b + 3 > 0 \wedge 27b^2 - 18ab + 56b - a^3 + 2a^2 - 19a + 29 = 0,$$

which gives the solution: $a = 1, b = -\frac{11}{27}$. Using the variable ordering $b \prec a \prec v \prec u$ we get the answer directly: $27b + 11 = 0 \wedge a - 1 = 0$.

Therefore we have found that the closest linear approximation to the polynomial $x^3 - x^2$ under the uniform norm on the interval $[-1, 1]$ is $x - \frac{11}{27}$. This is demonstrated in Figure 8.1.

8.2.1 Results

We have considered (8.1) with respect to two permissible variable orderings and now collect the results from this thesis: $a \prec b \prec v \prec u$ is given in Table 8.1 and $b \prec a \prec v \prec u$ is given in Table 8.2. These describe the possible CADs that are sufficient to solve (8.1), separated according to whether they are constructed using `ProjectionCAD`, QEPCAD, or `RegularChains`. Omitted CADs (that are not sufficient in this case to tackle (8.1)) include: TTICADs (which would be equivalent to an equational constraint CAD); layered sub-CADs (as the solution is 0-dimensional); layered variety sub-CADs; and the preconditioned versions of these theories.

It is clear from Tables 8.1 and 8.2 that the correct use of various advances in CAD can have a substantial effect on the complexity of the problem, particularly for projection and lifting algorithms.

Technique	Cells	Time	Section	Page
PL-CAD (Col)	54037	255.304	2.3	30
PL-CAD (McC)	54037	266.334	2.3	30
EC-CAD (f_3)	20593	65.856	2.4.4	40
EC-CAD (f_4)	22109	102.781	2.4.4	40
V-CAD (f_3)	8195	63.387	4.2	114
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GB-CAD (McC)	28501	128.533	6.2.2	201
GB-EC-CAD (g_4)	12513	55.749	7.1	249
GB-V-CAD (g_4)	**4171**	**53.251**	7.1	249
QEPCAD (full-cad no $\exists$)	54037	5.701	2.11	58
QEPCAD (no $\exists$)	1015	4.807	2.11	58
QEPCAD (full-cad)	349	4.782	2.11	58
QEPCAD	153	4.659	2.11	58
GB-QEPCAD (full-cad no $\exists$)	28501	5.198	6.2.2	201
GB-QEPCAD (no $\exists$)	73	4.669	6.2.2	201
GB-QEPCAD (full-cad)	625	**4.628**	6.2.2	201
GB-QEPCAD	**63**	4.801	6.2.2	201
RC-Rec-CAD	54037	327.421	2.5	43
RC-Inc-CAD	**29**	0.155	2.5.3	46
GB-RC-Rec-CAD	28501	219.280	6.2.2	201
GB-RC-Inc-CAD	**29**	0.148	6.2.8	220

Table 8.1: The Solotareff-3 problem — variable order $a \prec b \prec v \prec u$. The results are separated according to whether they are constructed using `ProjectionCAD`, QEPCAD, or `RegularChains`.

For the first variable ordering using `ProjectionCAD`, 54037 cells are reduced by 92.3% to 4171 cells in the sub-CAD of the appropriate variety generated from a Gröbner basis of the equational constraint polynomials. Similarly, for the second variable ordering with `ProjectionCAD`, 161317 cells are reduced by 99.0% to 1603 cells in the preconditioned variety sub-CAD.

There are some things to note on the results that have been mentioned in earlier sections. Out of the four equational constraints in the problem, only two are valid for use with either EC-CAD or V-CAD. Once a Gröbner basis has been computed, this reduces down to only one valid equation for use with GB-EC-CAD or GB-V-CAD. This is due to only a single polynomial involving the main variable: computing a Gröbner basis will never eliminate the main variable completely so we are always guaranteed at least one valid equation, but generally the main variable will be present in as few equations as possible.

Technique	Cells	Time	Section	Page
PL-CAD (Col)	161317	916.105	2.3	30
PL-CAD (McC)	154527	857.357	2.3	30
EC-CAD (f_3)	48475	175.139	2.4.4	40
EC-CAD (f_4)	63583	324.663	2.4.4	40
V-CAD (f_3)	19127	173.083	4.2	114
V-CAD (f_4)	25563	295.556	4.2	114
GB-CAD (Col)	10633	44.939	6.2.2	201
GB-CAD (McC)	10633	44.784	6.2.2	201
GB-EC-CAD (g_4)	4809	20.420	7.1	249
GB-V-CAD (g_4)	**1603**	**20.053**	7.1	249
QEPCAD (full-cad no $\exists$)	154527	8.249	2.11	58
QEPCAD (no $\exists$)	2065	4.785	2.11	58
QEPCAD (full-cad)	1063	4.832	2.11	58
QEPCAD	375	**4.687**	6.2.2	201
GB-QEPCAD (full-cad no $\exists$)	11319	4.836	6.2.2	201
GB-QEPCAD (no $\exists$)	53	4.715	6.2.2	201
GB-QEPCAD (full-cad)	251	4.796	6.2.2	201
GB-QEPCAD	**42**	4.816	6.2.2	201
RC-Rec-CAD	154527	1154.146	2.5	43
RC-Inc-CAD	**33**	0.202	2.5.3	46
GB-RC-Rec-CAD	10633	113.710	6.2.2	201
GB-RC-Inc-CAD	**33**	**0.161**	6.2.8	220

Table 8.2: The Solotareff-3 problem — variable order $b \prec a \prec v \prec u$. The results are separated according to whether they are constructed using `ProjectionCAD`, QEPCAD, or `RegularChains`.

When using QEPCAD, preconditioning proves useful for all variants of its algorithm[1]. Whilst the percentage savings from preconditioning are more modest than the savings for projection and lifting, it improves an already highly efficient algorithm and implementation.

The recursive `RegularChains` algorithm performs in an identical manner to projection and lifting by McCallum's operator, and is improved by preconditioning. The incremental algorithm provides quite startling results due to its ability to utilise all four equational constraints at once, which is not improved by preconditioning (as the Gröbner basis describes the same finite set of results). This is the optimal choice for all algorithms, even when compared against the two-dimensional partial CADs of QEPCAD.

The prominence of the incremental regular chains algorithm suggests that the most fruitful area of research in projection and lifting based CAD algorithms would be to try

[1] All QEPCAD timings include initialisation time, consisting of around two seconds per problem.

to utilise all equational constraints (extending the work on bi-equational constraints in [BM05]). This would allow for interaction with sub-CAD (within `ProjectionCAD`) or partial CAD (within QEPCAD) which could reduce this number even further.

8.3 Key Contributions

We now summarise the key contributions described in this thesis, followed by a summary of the author's individual contribution.

Chapter 3: Truth Table Invariant CAD

The new idea of truth table invariance was introduced, which considers a CAD with respect to a list of formulae rather than a set of polynomials. An algorithm was given that utilises equational constraints from each individual formula to simplify the projection and lifting stages of construction. This new algorithm was mathematically verified and shown experimentally to be hugely beneficial. This work was extended to interface with the incremental regular chains CAD algorithm from [CM12], which allows for the use of multiple equational constraints within each formula and more subtle case distinction to further improve the algorithm's efficiency. An application of CAD to branch cut analysis of complex identities was shown to be particularly suited for TTICAD.

The work in Chapter 3 was published in [BDE$^+$13], [BCD$^+$14], [EBDW13] and [ECTB$^+$14], and has been submitted in [BDE$^+$14].

Chapter 4: Cylindrical Algebraic sub-Decompositions

The idea of restricting the output of a CAD for a particular problem was formalised into the idea of a cylindrical algebraic sub-decomposition (sub-CAD). Further utilising the theory of equational constraints, the variety sub-CAD was defined to consist of all cells lying on a variety and an algorithm was given for its construction. Generalising the work in [McC93], an ℓ-layered sub-CAD consists of all cells of dimension $n - \ell + 1$ to n. Layered sub-CADs can be constructed directly or recursively, where the latter returns an unevaluated command to produce a further layer (which can be repeated until a full CAD is constructed). These ideas were combined with each other, and with TTICAD theory from Chapter 3, to further improve efficiency and reduce the size of the output CAD. A formal complexity analysis of variety sub-CADs and 1-layered variety sub-CADs showed that both offer a drop in the linear term in the double exponential for the computational

complexity. This theoretical saving was shown to equate to a practical increase in efficiency through a full implementation of the algorithms.

The work in Chapter 4 was first given in [WE13] and published in [WBDE14].

Chapter 5: Formulation of Problems

Variable ordering has been known to be of key importance to the complexity of CAD [BD07]. A new heuristic, `ndrr`, was introduced is particularly useful as a tie-breaker in conjunction with `sotd` from [DSS04]. Existing heuristics were investigated and shown to be useful for application to other formulation issues: equational constraint designation, formula decomposition, and incremental input ordering. Machine learning was used to select the optimal heuristic (from Brown's heuristic, `sotd`, and `ndrr`) for a large collection of examples, proving highly effective, and the experimental data was further used to indicate that Brown's heuristic performs the best of the three heuristics considered. The work in Chapter 4 inspired a new layered heuristic, which computes multiple 1-layered sub-CADs to predict the complexity of complete CADs. This was shown to be highly accurate, although at times costly.

The work in Chapter 5 was published in [BDEW13], [HEW$^+$14b], [HEW$^+$14a] and [EBDW14], and the work appearing in [WE13] has been submitted in [WEBD14].

Chapter 6: Mathematical Description

It was shown that the mathematical description of a problem, and how it is then processed for a CAD algorithm, can be a key factor that determines the feasibility of CAD construction. The idea of Gröbner preconditioning from [BH91] was investigated in depth, including a new effective heuristic for predicting its benefit, `TNoI`. A mathematical explanation for the behaviour of preconditioning was also given. The classic Piano Mover's Problem was investigated; whilst the original description of the problem is infeasible, a new expression was given that proves more suited for CAD. Although producing many cells, the new formulation was shown to have certain advantages over other approaches to this problem by CAD: working within the configuration space retains orientation information, and the formulation requires little geometric reasoning. A general approach to optimally expressing a problem mathematically for CAD was discussed.

The work in Chapter 6 has been published in [WBD12], [DBEW12] and [WDEB13].

Chapter 7: General Framework

It was demonstrated that whilst many of the concepts in this thesis can be combined together, this is not always the optimal choice. Due to restrictions in the applicability of certain algorithms, a sub-optimal formulation may need to be chosen when combining technologies. At worst, this sub-optimal formulation may prove less efficient than applying any of the technologies alone. This inspired a general approach to tackling a problem with CAD through a hierarchy of decisions (that may need to be traversed non-sequentially). A proof-of-concept piece of software was demonstrated, with the aim of helping a user utilise the recent advances in CAD theory.

Chapter 8: Future Work

Finally, a comprehensive list of directions in which this work could be extended was given. Each topic presented in this thesis has great potential for future work to build on the results discussed.

Author's Contribution

Work in this thesis has come from collaborations with researchers from the University of Bath and other universities. We briefly summarise the author's contribution:

Chapter 3: Truth Table Invariant CAD The author mainly contributed to discussions, experimentation, and analysis (in collaboration with the research group, McCallum, Chen, and Moreno Maza).

Chapter 4: Cylindrical Algebraic sub-Decompositions The work in this chapter was primarily the author's.

Chapter 5: Formulation of Problems The author contributed to discussions, experimentation, and analysis of the first section of work (in collaboration with the research group). The author contributed to designing and analysing the following section (in collaboration with Huang, Paulson and Bridge). The final section was primarily the author's work.

Chapter 6: Mathematical Description The work in this chapter was primarily the author's.

Chapter 7: General Framework The work in this chapter was primarily the author's.

8.4 Concluding Remarks

The aim of this thesis is to present a collection of advances within the theory of cylindrical algebraic decompositions and their applications. This has been achieved through five key topics: truth table invariant CAD; cylindrical algebraic sub-decompositions; formulation for CAD algorithms; mathematical description of problems; and how these concepts fit into a general framework. The topics have each been accompanied, where appropriate, with new definitions, formal algorithms, mathematical justification, implementations, experimental data, and scope for future research. The efficacy of these advances has been conclusively demonstrated (e.g. the Solotareff-3 example had 916.1 seconds of construction time reduced to 20.1 seconds) and disseminated through peer-reviewed articles in conference proceedings and journals.

This thesis has contributed to the field of CAD theory by providing a collection of advances that can significantly improve the efficiency of CAD algorithms in two ways. This is done both by improving the way a question is asked (Chapters 5 and 6) and tailoring the solution methodology to the precise formulation of the question (Chapters 3 and 4). Building on previous work in the field, these theories have allowed for a new implementation to compete with state-of-the-art software. With incorporation of the ideas of this thesis into optimised software even greater efficiency should be achievable. Although the work in this thesis can be considered alone, it is hoped that it will also be viewed as a platform for further improvements to the efficient construction of CADs tailored to particular problems in the future.

Appendices

Appendix A

Adjacency in CAD

We offer a survey of work concerning adjacency in cylindrical algebraic decompositions, as well as indicating implications on CAD algorithms and research. Whilst the subject of adjacency has not featured heavily in this thesis, it is of key interest and important to consider whilst developing CAD techniques. The current work into CAD adjacency will be described briefly, before suggestions of adaptations to the work of this thesis. This includes a new topological concept considered by the author in relation to sub-CADs.

A.1 Adjacency Background

Recall the two definitions of adjacency:

Definition A.1.
Given two disjoint cells D_1, D_2 of $\mathbb{R}^n$ we say they are **adjacent** if either:

(A1) their union, $D_1 \cup D_2$, is connected.

(A2) the cell of smaller dimension, (without loss of generality assumed to be D_2), is entirely contained in the closure of the larger-dimensional cell: $D_2 \subseteq \overline{D_1}$.

If D_1, D_2 are adjacent regions, we call the set $\{D_1, D_2\}$ an **adjacency**. If unclear, we can specify an **(A1)**-adjacency or **(A2)**-adjacency.

If $\{D_1, D_2\}$ is an **(A2)**-adjacency and D_2 is the cell of smaller dimension, we say D_2 is a **face** of D_1.

The following example demonstrates that whilst **(A2)** implies **(A1)**, the converse is not true.

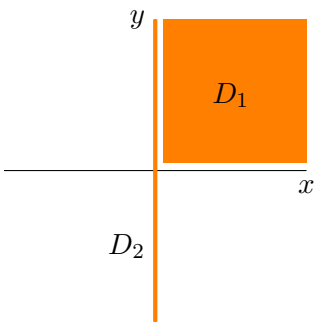


Figure A.1: An example of two CAD cells that are **(A1)**-adjacent, but not **(A2)**-adjacent.

Example A.1.
Let D_1 be the open first quadrant of the plane, defined by $x > 0 \wedge y > 0$. Let D_2 be the entire y-axis, defined by $x = 0$; these cells are shown in Figure A.1. Under the projection order $x \prec y$ these two cells are cylindrically arranged and both are semi-algebraic.

By definition **(A1)**, D_1 and D_2 are adjacent. However, the closure of D_1 is the closed first quadrant of the plane $(x \geq 0 \wedge y \geq 0)$ for which $\overline{D_1} \cap D_2 = (x = 0 \wedge y \geq 0) \neq \varnothing$, but $D_2 \nsubseteq \overline{D_1}$. Therefore **(A2)** deems these cells to be non-adjacent.

When discussing previous adjacency work we shall clarify which definition of adjacency is being considered. Often adjacency research will impose extra conditions on the CAD resulting in **(A1)** and **(A2)** being equivalent.

We distinguish specific types of adjacencies within a CAD.

Definition A.2.
Let $\{D_1, D_2\}$ be an adjacency in a CAD, $\mathcal{D}$, of $\mathbb{R}^n$. If D_1 and D_2 are both sections, we call $\{D_1, D_2\}$ a **section-section adjacency**.

As $\mathcal{D}$ is the union of stacks over cells in an induced CAD of $\mathbb{R}^{n-1}$, adjacencies can be divided into those between cells in the same stack, and those in different stacks. If D_1 and D_2 belong to the same stack we call $\{D_1, D_2\}$ an **intrastack adjacency**, and if they belong to different stacks we call $\{D_1, D_2\}$ an **interstack adjacency**.

Any CAD algorithm constructs cell indices, and knows the number of cells in every stack. As all intrastack adjacencies consist of a sector and the section either above or below it, it is simple to see if two cells in the same stack are adjacent (with respect to both **(A2)** and **(A1)**): intrastack cells are adjacent if and only if their final indices are consecutive integers.

Therefore the difficulty lies in interstack adjacencies, and in particular interstack section-section adjacencies (from which the entire interstack adjacencies can be calculated).

A.2 Properties Related to Adjacency

There are certain properties of CAD cells that are related to adjacency. These are not restricted just to cells of CADs and can be used for other decompositions or cell complexes.

Definition A.3.
Let $\mathcal{D}$ be a CAD of $\mathbb{R}^n$, and let D be a cell of $\mathcal{D}$ with dimension k. Recall that the **boundary** of D, ∂D, is equal to the difference of D and its closure: $\overline{D} \setminus D$.

We say that D is **boundary coherent** if its boundary is the union of cells of dimension less than or equal to $d-1$.

We say that D is **well-bordered** if its boundary is the closure of finitely many cells of dimension $d-1$.

We say that D is **boundary smooth** if for all points $p \in \partial D$, there exists an $\epsilon > 0$ such that the ball of radius ϵ centred at p is connected.

If every cell of $\mathcal{D}$ is boundary coherent, well-bordered, and boundary smooth then we say that $\mathcal{D}$ is a **strong cell decomposition**.

A strong cell decomposition is a very well-behaved CAD with respect to adjacency, and has appealing topological properties. It has not been shown which CAD algorithms produce a strong cell decomposition and it is being investigated by other researchers at the University of Bath.

A.3 Decidability of Adjacency in CAD [Arn79]

In [Arn79] the **(A2)** definition of adjacency is considered (and referred to as **incidence**). Arnon proves the following result which gives the decidability of adjacency:

Theorem A.1 ([Arn79])**.**
If the defining formulae and dimensions are known for each cell in a CAD then we can determine the incidences among cells.

Proof.
Let D_i be an i-cell and D_j be a j-cell, with $i < j$. We produce a sentence in the

elementary theory of real closed fields representing the statement "D_i is incident on D_j".

Let φ_i and φ_j be the defining formulae for D_i and D_j. Recall a **limit point**, x, of a set, S, is a point such that for every open ball of radius $\epsilon > 0$ centred at x contains a point $y \in S$ with $y \neq x$. Then the definition of **(A2)**–adjacency is equivalent to every point of D_i being a limit point of D_j (by the definition of closure).

The statement "every point of D_i is a limit point of D_j" can be expressed as the following sentence in the elementary theory of real closed fields:

$$\forall x \forall \epsilon \left[[\varphi_i(x) \wedge \epsilon > 0] \rightarrow \exists y \left[\varphi_j(y) \wedge 0 < d(x,y) < \epsilon \right] \right].$$

This is a statement in the elementary theory of real closed fields and therefore can be decided (for example by CAD-based quantifier elimination).

□

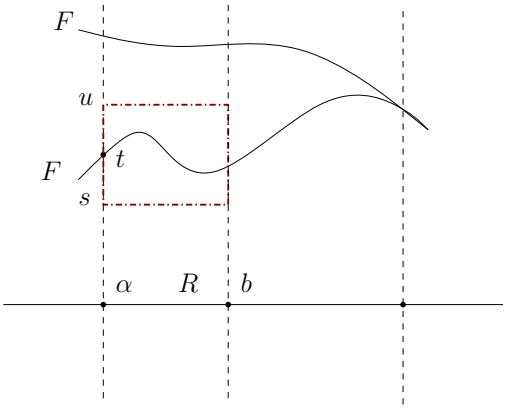
A.4 Adjacency Algorithms

We give a brief description of some of the work that has been done on algorithms for adjacency.

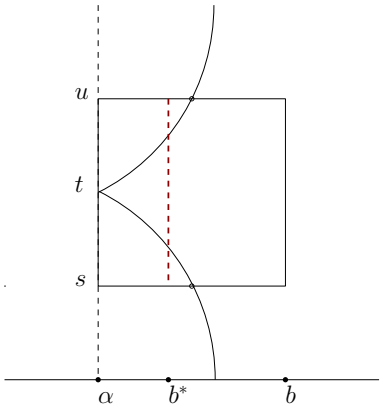
A.4.1 The Piano Mover's Problem [SS83b]

The authors of [SS83b] introduce a **well-based** condition that is similar to the stronger well-oriented condition required for Brown's projection operator. They prove that for well-based CADs **(A1)** and **(A2)** are equivalent.

The authors show that the compact cells within a well-based CAD form a regular cell complex (a well-studied topological structure). They use this along with the fact that every regular cell complex admits an incidence function to show the construction of an incidence function for a well-based CAD. They show explicitly how to compute incidence between cells of dimension n and $n-1$, which is all that is theoretically needed for the Piano Mover's Problem, using the number of roots over cells (computed by Sturm sequences). They describe a method to extend to cells of a lower dimension, although it requires fractional Laurent series and Newton approximation (with exponential complexity).



(a) Valid choice of u, s, b such that the number of sections adjacent to the section (α, t) is precisely the number of real roots of $F(b, y)$ in the interval (s, u).



(b) A case where $F(x, s)$ and $F(x, u)$ have real roots in $[\alpha, b]$. Using b^* instead of b would be a valid choice.

Figure A.2: Figures demonstrating the results from [ACM84b] relating to adjacency in the plane.

A.4.2 Adjacency in the Plane [ACM84b]

Following the description of the original CAD algorithm in [ACM84a], the authors discuss adjacency in [ACM84b], using definition **(A1)** and providing an algorithm to produce a CAD with adjacency information. They define a **proper CAD** recursively: there exists a polynomial $F \in \mathbb{Q}[x_1, \ldots, x_n]$ such that $V(F)$ is equal to the union of the sections of the CAD; and the induced CAD of $\mathbb{R}^{n-1}$ is proper.

Given a proper CAD of $\mathbb{R}^2$, with defining polynomial F, they prove a string of results that combine to form a straightforward algorithm to compute all section-section adjacencies. Given a 0-cell $\alpha \in \mathcal{D}'$, let R_1, R_2 be the cells to the immediate left and right of α. For each section (t, α) of F over α it is possible to find $s < t < u$ and $a < \alpha < b$ such that: t is the unique real root of $F(\alpha, y)$ in $[s, u]$; and $F(x, s)$ and $F(x, u)$ have no real roots in $[a, \alpha]$ nor $[\alpha, b]$. A correct and invalid choice are shown in Figure A.2. Given these conditions, the number of sections of $S(F, R_1)$ and $S(F, R_2)$ that are adjacent to the section (α, t) is equal to the number of real roots of $F(a, y)$ and $F(b, y)$ in (s, u). Further, the choice of a and b can be made universally for the entire stack over α.

For an input $A \subset \mathbb{Q}[x, y]$, it is simple to construct the CAD, $\mathcal{D}'$, of $\mathbb{R}^1$ for $P(x) = {}_{\mathbf{C}}\mathbf{P}(A)$. They prove that $A^* = \text{prim}\left(\prod_{0 \neq f \in A} f\right)$ is delineable over every cell in $\mathcal{D}'$, and that the union of the stacks defined by A^* gives a proper CAD of $\mathbb{R}^2$.

Together, these results gives an implementable, proven algorithm to construct a two-

dimensional CAD with adjacency information for all cells.

A.4.3 Algebraic Cell Decomposition [KY85]

This paper mainly deals with augmenting the algorithm of Ben-Or, Kozen and Reif (BKR) to provide a decomposition that, like CAD, distinguishes between connected components determined by the signs of a set of polynomials. This is done in approximately the same complexity of BKR: singly-exponential.

They work with cell complexes, so the closure of a cell is a union of cells and therefore **(A1)** and **(A2)** are equivalent. They construct a graph for the cell complex such that each node is a maximal connected component and the edges provide adjacency information.

A.4.4 Approximation and Incidence [Pri86]

Prill openly distinguishes between **(A1)** (which he names **adjacency**) and **(A2)** (which he names **incidence**). He uses a linear change of coordinates to guarantee the bounded cells form a cell complex and so has restricted application. With these transformed coordinates he builds an approximate decomposition and uses **incidence points** to identify incident cells.

A.4.5 Adjacency in Three Dimensions [ACM88]

The authors extend their work from [ACM84b] and consider **(A1)**. They define the boundary coherent property (which they call the **boundary property**), and show that for a CAD with this property **(A1)** and **(A2)** are equivalent. Further, a proper CAD will always have this property (but the converse is not necessarily true).

Considering three-dimensional CADs over proper CADs of $\mathbb{R}^2$, each boundary point of a cell must either be in the same stack as the cell or in some adjacent low-dimensional stack. Determining these interstack adjacencies separates into three cases depending on the possible dimension pairs: $\{1, 2\}$, $\{0, 1\}$, and $\{0, 2\}$ (with the latter two needing special consideration in the case of nullification). Nullification is a possibility (unlike in two dimensions) and can be avoided with a coordinate change, but this is undesirable. The authors give a method to ensure nullification can only occur on 0-cells, which allows an adaptation of the lifting stage to construct a CAD of $\mathbb{R}^3$ with boundary coherence.

With additional concepts such as basis-determined CADs and section boundary properties they provide an algorithm, `CADA3`, which constructs a CAD of $\mathbb{R}^3$ with boundary coherence along with a list of all adjacencies (finite and infinite) of the CAD.

A.4.6 Non-nullifying $\{0,1\}$-Adjacency and Local Box Adjacency [CM95, MC02]

These papers extend the work of [ACM88] looking at particular cases of the box algorithm.

In [CM95] the case of a non-nullifying $\{0,1\}$-adjacency is considered. It provides a theorem that allows a more efficient way to deal with these adjacencies. Further, it can be extended to four dimensions in certain cases.

The case of $\{0,1\}$-adjacencies is investigated further in [MC02], where the authors give a local algorithm for these adjacencies, building on the work of [CM95]. Efficient algorithms are given for cells in $\mathbb{R}^2$, $\mathbb{R}^3$, and $\mathbb{R}^4$ and a general algorithm is given for $\mathbb{R}^n$ that is unlikely to fail (and if so, can be rectified by an change of isolating interval). This work is, to the best of the author's knowledge, the most current research in CAD adjacency.

A.4.7 Using Adjacency Whilst Constructing CADs [Arn88]

In [Arn88] the author uses adjacency information to streamline the lifting stage of CAD by clustering cells together according to their signature with respect to the input polynomials (so that certain computations can be done only once for the whole cluster). The **(A1)** definition of adjacency is used, but as the output CADs from [ACM84b, ACM88] are being considered, this will be equivalent to **(A2)**. The idea of a graph representation and clustering is given and used throughout.

Given a set of polynomials $F = \{f_1, \ldots, f_m\} \subseteq \mathbb{Q}[x_1, \ldots, x_n]$ we represent a cell of a CAD $\mathcal{D}$ by a triple (I, σ, S) where I is the cell index, $\sigma = (\sigma_1, \ldots, \sigma_m) \in \{-1, 0, +1\}^m$ is the signature (sign of each polynomial in F on the cell), and S a sample point.

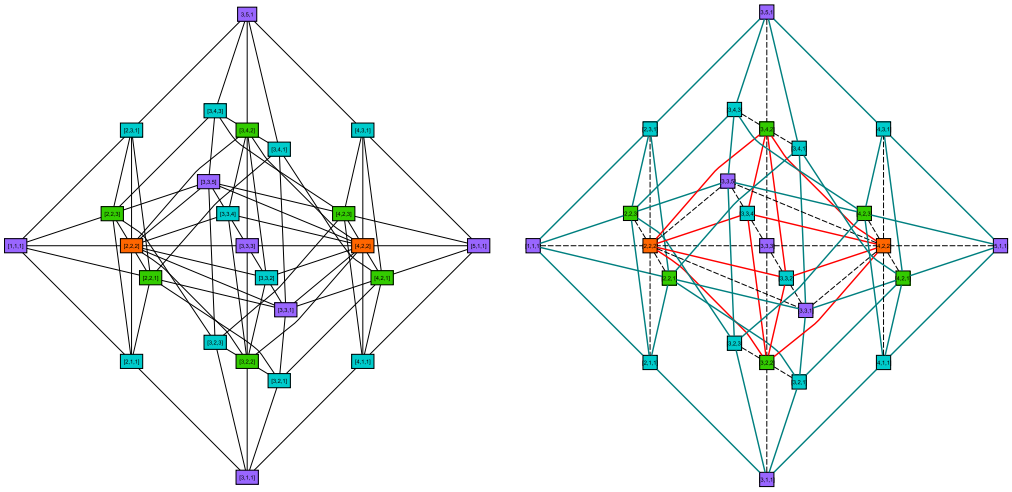
Definition A.4.
Let $F = \{f_1, \ldots, f_m\} \subseteq \mathbb{Q}[x_1, \ldots, x_n]$ and $\mathcal{D}$ an F-invariant CAD of $\mathbb{R}^n$. The **graph representation** of $\mathcal{D}$ is defined to be $G = (F, B, V, E, G')$ where:

F is the polynomials used to define $\mathcal{D}$.

B is a basis for $\text{prim}(F)$ such that $\mathcal{D}$ is a basis-determined CAD for B.

V is the set of vertices of the graph — all triples representing the cells in $\mathcal{D}$.

E is the set of edges of the graph. If (D_1, D_2) is an element of E, then D_1 and D_2 are adjacent in $\mathcal{D}$. If all adjacencies are represented by such an edge, G is called a **full graph**, else G is a **partial graph**.



(a) Graph representation. (b) Sign-invariance relation.

Figure A.3: The graph representation of the CAD of $F := \{x^2 + y^2 + z^2 - 1\}$ and the sign-invariance relation for F.

G' is the graph representation for the induced CAD $\mathcal{D}'$ if $r > 1$; and $G' = \varnothing$ if $r = 1$.

Definition A.5.
A collection of cells, C, of $\mathcal{D}$ is a **cluster** if the subgraph of G induced by C is connected. Equivalently, the union of cells in C is a region. The dimension of a cluster is the dimension of the largest cell in it. A partitioning of $\mathcal{D}$ into clusters is called a **clustering** of $\mathcal{D}$.

An equivalence relation R on the cells of $\mathcal{D}$ induces a clustering of $\mathcal{D}$ by computing the connected components of G when only edges satisfying R are considered. The **sign-invariance** relation is defined to be whenever two cells have the same signature; a **sign-invariant clustering** is one defined by a sign-invariance relation.

To give an example of a graph representation of a CAD, consider the unit sphere $F := \{x^2 + y^2 + z^2 - 1\}$. Figure A.3a gives the adjacency graph representation, and Figure A.3b gives the sign-invariance relation. The cells are coloured according to their dimension (in increasing order from 0-dimensional: orange, green, blue, purple). Figure A.3b includes clustering information: three clusters are produced corresponding exactly to the regions where F is positive, negative or vanishes. The blue edges connect cells that are adjacent and on which F is positive; the orange edges connect cells that are adjacent and on which F vanishes; the dashed edges connect cells that are adjacent but with differing sign for F (note there is only a single cell, that forms a trivial cluster, for

which F is negative).

The idea of using the sign-invariant adjacency information is as follows. Given an arbitrary PROJ(F)-invariant decomposition (not necessarily cylindrical) $\hat{\mathcal{D}}$ of $\mathbb{R}^{n-1}$ then we can extend it to a decomposition $\mathcal{D}^*$ of $\mathbb{R}^n$ by exactly the steps used in CAD for extension over a single cell. $\mathcal{D}^*$ may not be cylindrical, but if $\hat{\mathcal{D}}$ is algebraic then so is $\mathcal{D}^*$. Given a graph for a PROJ(F)-invariant CAD of $\mathbb{R}^{n-1}$ we can form a decomposition by taking the PROJ(F)-invariant clusters and lift as above to form an F-invariant decomposition of $\mathbb{R}^n$. This is summarised as follows:

1. If $n > 1$ call the algorithm recursively to build a graph for the induced CAD of $\mathbb{R}^{n-1}$.

2. (a) If $n > 1$ extend, over the maximal sign-invariant clusters of the induced CAD, to a graph for the CAD of $\mathbb{R}^n$.

   (b) If $n = 1$ build a graph directly

3. Construct additional adjacencies in $\mathbb{R}^n$. Cluster as appropriate.

This suggests a new definition for minimal CADs that could be useful.

Definition A.6.
We say an F-invariant decomposition $\mathcal{D}^*$ of $\mathbb{R}^n$ is a **(algorithmically) minimal decomposition** if during its construction no further clustering can be conducted.

We say an F-invariant CAD $\mathcal{D}$ of $\mathbb{R}^n$ is a **(algorithmically) minimal CAD** if the only clustering steps not used during its construction invalidate cylindricity.

Identifying algorithmically minimal CADs could be a fruitful research topic and comparing to algorithmically minimal decompositions could give further insight into what the cost of ensuring cylindricity is.

A.5 Future Work: Adjacency in sub-CADs

We discuss how the work in this thesis could apply to the adjacency theory described in the previous sections.

A.5.1 Adjacency in New CAD Algorithms

All the current CAD adjacency algorithms discussed in Section A.4 are designed for use with a projection and lifting CAD algorithm. There are no algorithms designed for

use with any of the regular chains algorithms, or for either a TTICAD or equational constraint CAD.

As deciding adjacency is a difficult process, but clearly useful, it would seem prudent to look at whether any properties of these new CAD algorithms and the CADs they produce are amenable to deciding adjacency. It may be that a particular algorithm can be shown to always produce a strong cell decomposition (Definition A.3), which automatically permits certain adjacency computations. Indeed, a tailored adjacency algorithm may be possible for certain new CADs.

A.5.2 Clustering in Adjacency Graphs and Minimality of CADs

In [Arn88] the definition of the graph representation of a CAD and sign-invariant clustering was given (reproduced in Definitions A.4 and A.5) where adjacent cells with identical sign signatures are clustered together. The algorithm described in [Arn88] then uses these clusters to simplify the CAD during the lifting phase.

This inspired the new Definition A.6 of algorithmically minimal decompositions. It would seem worthwhile to investigate this property to first identify algorithmically minimal CADs and then use this to motivate new advances. It is tempting to define minimality of a CAD related to the theoretically minimal CAD, but such a CAD may not be constructible by any algorithm. Definition A.6 is tied to an algorithm and so the algorithmically minimal CAD must be constructible.

A collection of algorithmically minimal CADs for a given algorithm would provide a ground truth to compare other algorithms to, along with allowing further insight into concepts like variable orders. This would avoid any artefacts of the algorithms' implementations having an impact on the results.

A.5.3 Adapting Adjacency in sub-CADs

Previous work on adjacency in CAD has had limited impact due to both the complexity of the algorithms (for $\mathfrak{D}$ cells, $O(\mathfrak{D}^2)$ adjacencies will need to be considered, of which some will be non-trivial) and necessary conditions such as boundary coherence or well-borderedness (which need to not just hold, but be explicitly shown to hold).

There is hope that the sub-CAD techniques introduced in Chapter 4 might help. A sub-CAD is a subset of the cells in a CAD and so the issue of complexity of an adjacency algorithm is immediately reduced, although still present. The issue of boundary coherence or well-borderedness is also still present but reduced. Given a TTICAD that fails the well-orientedness condition there is a chance that a sub-TTICAD avoids the trou-

blesome cells and so constructs without theoretical failure. The same possibility exists with sub-CADs and the adjacency conditions from Section A.2: if the cells that violate one of those conditions are not contained in the sub-CAD then an existing adjacency algorithm can be applied.

There is an additional benefit to constructing a layered sub-CAD. In [SS83b] the authors give an explicit algorithm for computing adjacencies of n and $(n-1)$ dimensional cells, pointing out that comparing cells of lesser dimension introduces further complication. Therefore a 2-layered sub-CAD (but not a 2-layered variety sub-CAD) would allow application of the simpler form of this algorithm. It also suggests that the $\{n, n-1\}$ adjacencies are somehow "simpler" than other adjacencies. This should be investigated further to see if adjacencies behave differently depending on the layers being considered, and if the restriction to a variety sub-CAD affects this relation.

A.5.4 Topology: ℓ-dimensionally Path Connected

We attempt to relate the concepts arising within layered sub-CADs to topological properties. Recall the definition of an ℓ-dimensional ball:

Definition A.7.
The **ℓ-dimensional ball** centred at the point $\alpha \in \mathbb{R}^\ell$ of radius $\epsilon > 0$, denoted by $B_\epsilon^{(\ell)}(\alpha)$, is defined to be:

$$B_\epsilon^{(\ell)}(\alpha) := \left\{ x \in \mathbb{R}^\ell \mid |x - \alpha| < \epsilon \right\} \tag{A.1}$$

The idea of spaces being connected by paths is well-defined and studied within Topology, with the following definition being the basis of path-connectedness.

Definition A.8. [Wil04]
A space X is **pathwise connected** if and only if for any two points x and y in X, there is a continuous function $f : [0,1] \to X$ such that $f(0) = x$, $f(1) = y$.

However, path-connectedness can be perhaps deceptive as the following example shows.

Example A.2.
Consider the plane, $\mathbb{R}^2$, and the four open quadrants labelled clockwise from the positive quadrant. Let X be the first quadrant and Y the third quadrant, as shown in Figure A.4.

The closures, $\overline{X}$ and $\overline{Y}$, are path connected. In particular, $\overline{X} \cap \overline{Y} = \{(0,0)\}$ so any path between points in separate quadrants must pass through the origin.

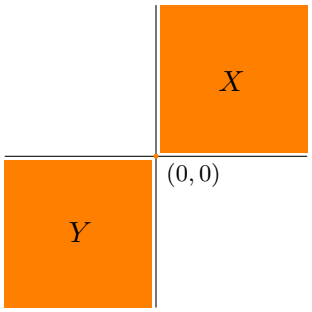


Figure A.4: Two quadrants of the plane that are path connected through the origin.

For practical applications of CAD we often want a stronger condition. Unaware of a formal definition in Topology, we create such a definition here:

Definition A.9.
A space X is said to be **ℓ-dimensionally pathwise connected** if for any two points x and y in X, there is $\epsilon > 0$ and a continuous function $f : B_\epsilon^{(\ell)}(\mathbf{0}) \times [0,1] \to X$ such that $f(\mathbf{0}, 0) = x$ and $f(\mathbf{0}, 1) = y$.

Clearly 0-dimensionally pathwise connected is equivalent to the definition of pathwise connected given in Definition A.8. Informally, 1-dimensionally and 2-dimensionally path-connected spaces are those in which we can connect any two points by a deformation of a non-trivial ribbon or cylinder, respectively.

Consider Example A.2. We see that whilst the quadrants are 0-dimensionally path-connected, they are not 1-dimensionally path connected (unlike the closure of two adjacent quadrants).

With Definition A.9 we can consider connectivity of an ℓ-layered sub-CAD.

Theorem A.2.
Let $\mathcal{D}$ be an ℓ-layered CAD. Then each path-connected component of $\mathcal{D}$ is, at least, $(n - \ell + 1)$-dimensionally path connected.

Proof.
Let x and y be in the same path-connected component of $\mathcal{D}$, say X, and let $f : [0,1] \to X$ be a path connecting x and y.

As $\mathcal{D}$ is ℓ-layered, X is comprised of a union of a finite number of cells, each with dimension in the range $n - \ell + 1 \leq d \leq n$. For each cell D_i, let ϵ_i be the smallest distance from a point on the image of f to the boundary of the closure of D_i. As each cell is open, this value is non-zero and an $(n - \ell + 1)$-dimensional ball of radius ϵ_i can surround every point of $f([0,1])$ in D_i without intersecting the boundary of $\overline{D_i}$.

Choosing $\epsilon > 0$ such that $\epsilon < \min(\epsilon_1, \ldots, \epsilon_m)$ therefore proves that X is $(n - \ell + 1)$-dimensionally path-connected.

□

The idea of ℓ-dimensional path connectedness can also transfer to layered variety sub-CADs, although care needs to be taken with dimensions to account for the co-dimension of the variety.

It would seem that this new definition of path connectedness is well-suited for robot motion planning: a solid three-dimensional object cannot move between two three-dimensional regions by passing through just a 0-dimensional or 1-dimensional cell, and so 2-dimensional path connectedness is required. Dimensional path connectedness does not guarantee the presence of a valid path however, only the topological possibility (e.g. something of 10m width can topologically fit through a 1cm hole but cannot geometrically).

The work on the Piano Mover's Problem in Section 6.3 showed that it is now feasible to construct CADs for motion planning problems, albeit only for the most simple cases. Combined with sub-CAD techniques, as described in Section 6.3.9, the construction is simplified and the main issue is that of adjacency. An algorithm that constructs a graph representation of a layered variety sub-CAD with respect to the ℓ-dimensional path connectedness relation would be sufficient to solve this problem.

Appendix B

A Repository of CAD Problems

In the process of investigating various properties of CADs, it seemed important to have a large collection of examples to consider. This prompted the creation of a CAD repository which was opened for public use in [WBD13] and is available online at [Wil12].

B.1 Motivation and Practical Considerations

Due to the high complexity of CAD (Section 2.6) it can be difficult to find feasible problems to test.

As a CAD is a representation of the underlying structure of a system of polynomials, random examples behave quite differently to those sourced from applications or pre-defined problems.

Because of these two facts, the majority of problems were sourced from various key papers in the CAD literature. These currently include: [CMXY09], [Laz88], [McC88], [CMA82], [DSS04], [CH91], [Hon90], [Ach56], [Dav86], [BH91], [AM88], [Dav11], [BG06], [BDE$^+$13].

Whilst this approach avoids the creation of random examples, it is not without its own drawbacks. The examples in the literature are generally those well-suited to particular existing techniques. With advances in CAD technology like those mentioned in this thesis, problems that were previously considered 'hard' may become simple to tackle. Also, if a new technique is suited for problems of a certain form (for example TTICAD in Chapter 3) then there may not be examples in the literature appropriate to test it with. This is compensated by the creation of new examples and their inclusion into the example bank.

For each example sourced, the following are provided:

- The full statement of the problem (with quantifiers if appropriate);
- A list of free and quantified variables, along with a suggested variable ordering if one is given in the original statement;
- The best achieved number of cells (see Section B.2);
- Notes on the problem and the original source;
- Input for both Maple and Qepcad.

Since its creation and public launch in [WBD13], the repository has grown to contain a variety of examples, although it is still small compared to other example banks such as nlsat. Hopefully it will continue to expand and become a useful resource for researchers of CAD theory.

B.2 Theoretical Questions

Although a rather simple database of examples, certain questions arose during its creation that have proven interesting and significant.

On a broad level, the main question to be considered is what constitutes a new CAD problem. It seems fairly clear that reordering the variables in a problem does not fundamentally change the problem (unless the ordering is dictated by a quantifier elimination problem). However, for example, preconditioning input can produce a drastically different CAD.

This highlights a hierarchy of specificity for CAD problems, that was discussed in Chapter 7. Consider the Piano Mover's Problem discussed in Section 6.3. At the highest level we have a completely abstract problem: "can a ladder fit through a corridor". This translates (in a variety of ways, as discussed) into a "logical" problem, which leads to a semi-algebraic variety. The semi-algebraic variety in question can be formulated into an expression of polynomials (again, possibly in multiple ways). This equation can then be "oriented" through the choice of a variable order before, finally, a CAD can be produced (after deciding invariance conditions, sub-CAD techniques and so forth).

There is a choice of which part of this hierarchy we describe in our repository, and it seems that the translation of the logical problem into an expression of polynomials is a sensible thing to consider. All formulations derived from such an expression will be related, in that (after possible re-orientation) cells from CADs of different formulations will be subsets or supersets of each other. However, a different logical formulation (such as Section 6.3.4 compared to [Dav86]) will produce a completely different CAD.

Including a field that showed the minimal number of cells for a given problem is desirable - it gives an indication of the difficulty of the CAD problem. However, it is not obvious what "minimal" should stand for. There are theoretically minimal CADs for problems that cannot be constructed by any known algorithm. Therefore, the field was changed to be "best achievable number of cells" (with information on how to obtain this number where appropriate).

The idea of minimality of CADs is a hugely complex area without even a well-defined question. Work in [Bro98] discusses the idea of simplifying a CAD post-production according to truth value to minimise its complexity. Certain lifting techniques can be thought of as methods of minimising complexity during the construction phase, and restriction of output (for example sub-CADs and partial CADs) can be thought an extreme case. Many of these ideas are being considered by other members of the research group.

Appendix C

Implementations

The implementation of the work in this thesis is discussed. Certain issues that occurred during the implementation of various algorithms, but which were not related to the theory, are given along with descriptions of their solutions.

Implementation of the projection and lifting CAD algorithms in the `ProjectionCAD` module for Maple was not conducted by the author, but by Dr. England of the research group. Details are given in [Eng13a, Eng13b, EWBD14] and the work is summarised here due to its relevance to the theory and experimentation of this thesis.

Details of the author's implementation of sub-CAD algorithms in `ProjectionCAD` were originally described in [WE13] (describing the original `LayeredCAD` extension).

All Maple packages described in this appendix are available freely for download from the author's website[1]. The CADassistant tool is available freely for download from the author's GitHub repository[2].

C.1 The `ProjectionCAD` Module

Many of the algorithms discussed in this thesis are from the `ProjectionCAD` module in Maple. This was created by another member of the research team at Bath to provide a projection and lifting CAD algorithm that is customisable and for which we can post-process the output within Maple. The implementation is discussed in detail in [Eng13a, Eng13b, EWBD14], and we briefly discuss it here.

The `ProjectionCAD` algorithms are all projection and lifting based and follow the CAD algorithms of [Col75, McC85, McC99, Bro01], which cover construction by the

[1] `http://www.cs.bath.ac.uk/~djw42`

[2] `http://www.github.com/DavidJohnWilson/CADassistant`

various projection operators (using the `CADFull` command along with the `method` parameter) along with utilising equational constraints (using the `ECCAD` command). These are extended using the theory of Chapter 3 to include the `TTICAD` algorithm. There are also algorithms to use the various heuristics detailed in Chapter 5.

Whilst the CAD algorithms are projection and lifting based, `ProjectionCAD` is built over the `RegularChains` module (and the `SemiAlgebraicSetTools` sub-module), as described in [EWBD14]. Cells are represented by regular chains, and lifting is done using the `RegularChains` stack generation procedure.

One particular property of the `ProjectionCAD` module compared to other projection and lifting implementations is that it includes the improved equational constraint lifting that follows from [McC99] but was not explicitly noted until [BDE+13]: the final lifting stage needs to only be with respect to the equational constraint as opposed to the entire input set. This means that the `ECCAD` can sometimes perform better than other equational constraint implementations (such as QEPCAD). However `ProjectionCAD` does not implement the theory of partial CAD or contain a quantifier elimination procedure.

C.2 Algorithms for sub-CADs in the `ProjectionCAD` Module (in MAPLE)

In developing the theory of cylindrical algebraic sub-decompositions (described in Chapter 4) it was important to have an implementation of the algorithms described to allow for comprehensive experimentation. Algorithms to construct variety, layered (direct and recursive), and layered variety sub-CADs were implemented by the author in MAPLE as an extension of the `ProjectionCAD` package. The corresponding algorithms for sub-TTICADs (Section 4.4.2) are also given. This explanation was first given in the technical report [WE13].

Originally provided as a separate package, `LayeredCAD`, the following user-level commands are available:

- `VCAD([f,G],vars);`
- `VCADLiftOverLowCAD(lowCAD, equCon, vars);`
- `VTTICAD(Phi,vars);`
- `LCAD(F,L,vars);`
- `LCADRecursive(F,vars,C,LD);`

- `LTTICAD(Phi,L,vars);`
- `LCADDisplay(LCAD);`
- `LVCAD([f,G],L,vars);`
- `LVTTICAD(Phi,L,vars);`

The functions also allow further options through additional input parameters: for example those constructing sub-CADs allow for an `output` parameter of `list`, `listwithrep`, or `piecewise` (which is discussed in Section C.2.4).

We discuss briefly the implementations of these procedures, highlighting points of interest.

C.2.1 Variety sub-CAD Procedures

The variety sub-CAD procedures were straightforward to implement over the `ProjectionCAD` package, and `VCAD` follows Algorithm 4.1.

Upon calling `VCAD`, the input polynomials are projected and an $(n-1)$-dimensional CAD is created using the standard CAD algorithms in `ProjectionCAD`. The important step is then a call to `VCADLiftOverLowCAD` which lifts from an $(n-1)$-dimensional CAD to the variety. This is simple (assuming the input satisfies the requirements of Algorithm 4.1): for each cell of the lower-dimensional CAD a stack is generated with respect to the equational constraint (defining the variety) and if this contains more than one cell, the even indexed cells are retained.

C.2.2 Layered sub-CAD Procedures

Constructing a layered sub-CAD requires a little more care to ensure that the correct dimension cells are returned. Underlying all algorithms is a check whether a cell is of sufficient dimension to produce cells for the specified layered sub-CAD. This is determined using the following formula:

$$\dim(D) = \sum_{i \in D.\texttt{index}} (i \mod 2)\,.$$

A valid cell for an ℓ-layered sub-CAD of $\mathbb{R}^n$ must have dimension greater than or equal to $n+1-\ell$. Similarly, when considering a cell in $\mathbb{R}^k$, then it can only contribute a cell to an ℓ-layered sub-CAD of $\mathbb{R}^n$ if the cell has dimension greater than or equal to $k+1-\ell$.

This check is implemented within a subprocedure, `IsCellLLayeredDim`, which is simple to implemented in Maple. Constructing a layered sub-CAD using the `LCAD` command follows Algorithm 4.3 closely, using the `IsCellLLayeredDim` check repeatedly.

Of more interest is the `LCADRecursive` command, which constructs an ℓ-layered sub-CAD recursively, with respect to ℓ, following Algorithm 4.4.

The input for `LCADRecursive` an $(\ell - 1)$-layered sub-CAD `LD` and the corresponding list of terminating sections `C` (as well as the input polynomials and variable ordering). Both `C` and `LD` can be empty lists, which will produce a 1-layered sub-CAD for F, and this is the recommended initialisation. It is intended that the user should never manually enter `C` and `LD` (other than as empty lists), but they should be automatically generated by previous calls to the algorithm.

The algorithms then propagate the next layer of the CAD from the cells in `C` and give a pair of outputs (which can be assigned to multiple variables):

```
> A,B:= CADRecursiveLayered(F,vars,C,LD);
        LD', %CADRecursiveLayered(F,vars,C',LD')
```

The first output, `LD'`, is a layered CAD for `F` and `vars` of precisely one layer more than `LD`. The second output is a recursive call that can be used to produce a layered CAD with one more layer (and another recursive call). This recursive call is rendered inert by the Maple identifier `%`, but can be evaluated using the `value` command.

```
> A',B':= value(B);
        LD'', %CADRecursiveLayered(F,vars,C'',LD'')
```

In the current implementation the recursive call, `B`, is given in full detail, with `C'` and `LD'` explicitly printed. This is less than ideal, as the cells and layered CADs are often very large and complicated lists. To this extent it is recommended to assign the call 'quietly' (using `:` to terminate the statement rather than `;`) and then evaluate separately. It is hoped in future versions of the package this will be avoided through explicit type declaration (as is planned for the whole `ProjectionCAD` package).

C.2.3 Combined sub-CAD Procedures

Constructing layered manifold sub-CADs, or sub-TTICADs is a straightforward combination of the implemented sub-CAD algorithms, along with the TTICAD procedures provided within `ProjectionCAD`. It is not possible to construct recursive layered sub-TTICADs at the moment, as the process of constructing a layered sub-TTICAD is not uniform: the initial projection and final lifting stages are different from the others.

$$|x| := \begin{cases} x & x \geq 0 \\ -x & x < 0 \end{cases}$$

(a) Maple GUI Output.

```
                { x          0 <= x
|x| := piecewise(
                { -x         x < 0
```

(b) Maple Command-line Output.

Figure C.1: The result of the `|x|:=piecewise(x<0,-x,x>=0,x)` command in Maple.

C.2.4 `LCADDisplay` and `piecewise` Output

It is notably difficult [CDM+09] to display a CAD in a clear and concise way, and communicating a sub-CAD presents extra challenges. It is important to communicate to the user of a sub-CAD algorithm the following items:

- The cells within the sub-CAD (represented by a sample point and index), preferably with a clear representation of the semi-algebraic set they define;
- The structure and relations of these cells, highlighting their cylindrical nature;
- An indication of where cells have been discarded in the creation of the sub-CAD.

The `piecewise` construct in Maple is used to display piecewise functions, such as the absolute value function, in a typographic style. Figure C.1 shows the result of defining the absolute value function (with `|x|:=piecewise(x<0,-x,x>=0,x)`) with this construct: Figure C.1a shows the formatted output available in the Maple graphical user interface; Figure C.1b shows the output available in the Maple command-line interface.

In [CDM+09] the authors demonstrated how the `piecewise` command could be used to display geometrical decompositions in a meaningful manner. They provide usage of this construct for comprehensive triangular decompositions, cylindrical algebraic decompositions, and real triangular decompositions. Furthermore, they demonstrate usage of inert computations (designation in Maple with the prefix of `%` and evaluation with the `value` command) when discussing lazy real triangular decompositions [CDM+10].

If a layered CAD has been constructed using the `listwithrep` formulation then it can be displayed in an informative tree-like structure using `LCADDisplay`. This outputs a Maple `piecewise` structure that gives an intuitive description of the layered CAD. Whenever a branch has been terminated a placeholder is given.

A simple example is given in Figure C.2a. This can be compared to Figure C.2b which shows the equivalent complete CAD in piecewise format. We see that the layered CAD displayed omits all information regarding the cylinder above $y = 0$ as this is unnecessary

```
  > LD,RLD:=LCADRecursive({x+y-1,y},[x,y],[],[],output=listwithrep):
  > LCADDisplay(LD);

{{ [regular_chain, [[-1, -1],[1, 1]]]       x < -y + 1
{{
{{            ["*********"]               branch = truncated       y < 0
{{
{{ [regular_chain, [[-1, -1],[3, 3]]]       -y + 1 < x
{
{                          ["*********"]                  branch = truncated
{
{{ [regular_chain, [[1, 1],[-1, -1]]]       x < -y + 1
{{
{{            ["*********"]               branch = truncated       0 < y
{{
{{ [regular_chain, [[1, 1],[1, 1]]]         -y + 1 < x
```

(a) Usage of `LCADDisplay` for a piecewise layered CAD

```
> CADFull({x y-1,y},[x,y],method=McCallum,output=piecewise);

{{ [regular_chain, [[-1, -1],[1, 1]]]        x < -y + 1
{{
{{ [regular_chain, [[-1, -1],[2, 2]]]        x = -y + 1        y < 0
{{
{{ [regular_chain, [[-1, -1],[3, 3]]]        -y + 1 < x
{
{  { [regular_chain, [[0, 0],[0, 0]]]          x < 1
{  {
{  { [regular_chain, [[0, 0],[1, 1]]]          x = 1           y = 0
{  {
{  { [regular_chain, [[0, 0],[2, 2]]]          1 < x
{
{{ [regular_chain, [[1, 1],[-1, -1]]]        x < -y + 1
{{
{{  [regular_chain, [[1, 1],[0, 0]]]         x = -y + 1        0 < y
{{
{{  [regular_chain, [[1, 1],[1, 1]]]         -y + 1 < x
```

(b) Full piecewise CAD

Figure C.2: The piecewise output for a sub-CAD and complete CAD produced with `ProjectionCAD`.

for a 1-layered CAD, along with the sections $x = 1 - y$ when $y > 0$ or $y < 0$. However, and importantly, it still indicates that cells are present in these branches, although no further details (such as the number of missing cells) are given as these are not computed. Obviously this is a near-minimal example, and the added clarity of representing a sub-CAD in this manner becomes even more pronounced and useful for larger sub-CADs.

C.3 Machine Learning Test Scripts

The problems chosen for the experiments in Section 5.3 [HEW+14b, HEW+14a] were all chosen from the NLSAT database, which provides descriptions of existential problems in the QEPCAD format. Construction of the CADs (and partial CADs) would be done within QEPCAD and thus require no adaptation of the input. The computation of the feature vector or heuristics could not be completed within QEPCAD as it is not a computer algebra system, so MAPLE and `ProjectionCAD` were used for these purposes.

The author had already written a PYTHON script to convert polynomials in the QEPCAD format to the MAPLE convention[3] (and vice versa) and this was expanded as necessary.

The resulting script, `CADqepcadtomaple.py`, takes an input file and output destination and performs the following:

1. Extracts the polynomials from the QEPCAD input formula and converts them into MAPLE polynomials.

2. Extracts the variable ordering from the QEPCAD input and converts it into a MAPLE ordering[4].

3. Constructs MAPLE code to compute the feature vector for the problem, which requires only basic MAPLE functions such as `degree`, `coeffs` and `nops`.

4. Constructs MAPLE code to compute the variable ordering choice for Brown's heuristic, `sotd` and `ndrr` using the `VariableOrderingHeuristic` procedure from `ProjectionCAD` (also reversing the ordering choices to align with QEPCAD's convention).

[3]The main difference in notation is that QEPCAD indicates multiplication by whitespace, whilst in MAPLE an asterisk is used. Therefore `2 x^3 y^2` would be converted to $\texttt{2} * (\texttt{x}^3) * (\texttt{y}^2)$.

[4]The ordering conventions are reversed, so that $z \prec y \prec x$ is represented as $(\texttt{z}, \texttt{y}, \texttt{x})$ in QEPCAD and as $[\texttt{x}, \texttt{y}, \texttt{z}]$ in MAPLE.

```
(x0,x1,x2)
0
(E x0)(E x1)(E x2)[[((x0 x0) +
   ((x1 x1) + (x2 x2)))=1]].
go
go
go
d-stat
go
finish
```

(a) Quantified input.

```
(x0,x1,x2)
3
[[((x0 x0) + ((x1 x1) + (x2 x2)))=1]].
go
go
d-proj-factors
d-proj-polynomials
go
d-fpc-stat
go
finish
```

(b) Unquantified input.

Figure C.3: The QEPCAD inputs for the quantified and unquantified version of a simple problem.

5. Writing the above commands to the output destination, which can then be read into any instance of MAPLE (in this case, command-line interface) to output the feature vector and three heuristic choices.

Following application of this script, the feature vector and heuristic choices for each example could then be easily computed. Ideas from this script were subsequently used in CADASSISTANT.

The input into QEPCAD also had to be prepared appropriately for the quantified and unquantified cases. Sample input files are shown in Figure C.3.

C.4 The CADASSISTANT Program (in PYTHON)

We describe the implementation of CADASSISTANT, which is discussed in Section 7.3.

The prototype of CADASSISTANT is implemented in PYTHON and can be run from the command line with either `interactive` or `manual` mode specified:

```
$ python CADassistant.py interactive
$ python CADassistant.py manual
```

The `interactive` and `manual` modes are simply different approaches to deciding formulation choices such as those discussed in Chapter 5.

In `manual` mode a list of questions are asked requiring the user to specify the construction method, invariance condition, sub-CAD techniques (if applicable), formula decomposition (if applicable), and equational constraints (if applicable). The `interactive`

method instead asks the user a sequence of questions to assist or automatically make these choices. This may require the user to paste commands into MAPLE (such as heuristic computations) and copy the output back into CADASSISTANT. These decisions are then encoded into an instance of a CAD object based on one of the CAD classes detailed in the following section.

C.4.1 CAD Classes

A basic `CadProblem` class is used to create an object for each problem to store important information. It contains instance variables to store the name, polynomials, and variables of the problem, and methods to output strings containing information related to the CAD.

1. `CadProblem`(`name`, `polys`, `variables`):
   - Variables:
     - `name`: string;
     - `polys`: list of strings;
     - `variables`: list of strings.
   - Methods:
     - `printCAD`(): returns a string describing the CAD (including name, polynomials, and variables);
     - `listOfPolys`(): returns a comma-separated list of the polynomials (delimited by `[` and `]`);
     - `listOfVariables`(): returns a comma-separated list of the variables (delimited by `[` and `]`);

Inheriting from the `CadProblem` class is the `CadProblemMethod` class which specifies which algorithm should be used for the given problem. This information is stored in extra variables, and an additional method creates a string with the CAD acronym (using the acronyms listed in the CAD Dictionary in Appendix D).

2. `CadProblemMethod`(`name`, `polys`, `variables`, `constr`, `inva`, `subCAD`) (inherited from `CadProblem`):
   - Variables:
     - `constr`: string (construction method; `pl` or `rc`);
     - `inva`: string (invariance; `si`, `oi`, `ec`, or `tti`);

- `subCAD`: string (subCAD type; `m`, `l`, or `lm`).

- Methods:
  - `printCADproblem`(): returns a string describing the CAD (including name, polynomials, variables, and CAD acronym);
  - `CADacronym`(): returns a string describing the CAD using an acronym (as described in Appendix D).

If the CAD to be constructed is a truth table invariant CAD, the `CadTTICAD` class can be used. This is inherited from `CadProblemMethod` and contains variables to describe the formulae and designated equational constraints. All numbering is done with respect to the order of the polynomials in the `poly` variable, and methods are used to check that the designation and formula decomposition is valid.

3. `CadTTICAD`(`name`, `polys`, `variables`, `constr`, `inva`, `subCAD`, `clauses`, `eqcons`) (inherited from `CadProblemMethod`):

   - Variables:
     - `clauses`: list of lists of integers (identifying clauses from the order of the polynomials in `polys`);
     - `eqcons`: list of lists of integers (identifying the equational constraint, if any, in each clause).

   - Methods:
     - `printTTICAD`(): returns a string describing the CAD (including name, polynomials, variables, CAD acronym, clause decomposition, and equational constraint designation);
     - `printTTICADClauses`(): returns a string describing the clauses and designated equational constraints (corresponding to the order of the polynomials in `polys`);
     - `setClauses`(`clauses`): sets the clauses according to a list of lists of integers (calls `checkClausesInp`(`clauses`) to check the clauses given are valid, and then calls `setClauses`(`clauses`));
     - `setEqCons`(`eqcons`): sets the equational constraint designations according to a list of lists of integers (calls `checkEqConsInp`(`clauses`) to check the equational constraints given are valid, and then calls `setEqCons`(`clauses`)).

C.4.2 Output Formats

The output format of CADassistant depends on which algorithm is required. Currently output can be given for Maple and Qepcad. The conversion is done using sections of the scripts described in Section C.3 and the output can be copied into the appropriate system to construct the requested CAD.

Appendix D

CAD Dictionary

A reference list of the various CAD acronyms that are used throughout this thesis. In particular, the various composed forms of CAD are given in their acronym and full descriptive form.

D.1 A Dictionary of CAD Acronyms

We provide a reference list of abbreviations and definitions for various forms of CAD.

CAD: **C**ylindrical **A**lgebraic **D**ecomposition as defined in Definition 2.14.

SICAD: **S**ign-**I**nvariant **CAD** as defined in Definition 2.16.

OICAD: **O**rder-**I**nvariant **CAD** as defined in Definition 2.25.

PL-CAD: **P**rojection and **L**ifting based **CAD** using one of the following projection operators:

Collins: [Col75] as defined in Definition 2.22;

Collins–Hong: [Hon90] as defined in Definition 2.23;

McCallum: [McC85] as defined in Definition 2.24;

Brown–McCallum: [Bro01] as defined in Definition 2.27.

EC-CAD: **E**quational **C**onstraint **CAD** [McC99] described in Section 2.32.

P-CAD: **P**artial **CAD** [CH91] described in Section 2.4.2.

RC-CAD: **R**egular **C**hains **CAD** using either:

RC-Rec-CAD: Recursive algorithm [CMXY09] described in Section 2.5.2;

RC-Inc-CAD: Incremental algorithm [CM12] and described in Section 2.5.3.

TTICAD: Truth **T**able **I**nvariant **CAD** [BDE+13, BDE+14, BCD+14], defined in Definition 3.2, and described in Chapter 3.

L-CAD: Layered sub-**CAD** [WBDE14], defined in Definition 4.4, and described in Section 4.3.

V-CAD: Variety sub-**CAD** [WBDE14], defined in Definition 4.3, and described in Section 4.2.

LV-CAD: Layered **V**ariety sub-**CAD** [WBDE14], defined in Definition 4.6, and described in Section 4.4.

L-TTICAD: Layered **T**ruth **T**able **I**nvariant sub-**CAD** [WBDE14] and described in Section 4.4.2.

V-TTICAD: Layered **T**ruth **T**able **I**nvariant sub-**CAD** [WBDE14] and described in Section 4.4.2.

LV-TTICAD: Layered **V**ariety **T**ruth **T**able **I**nvariant sub-**CAD** [WBDE14] and described in Section 4.4.2.

Table D.1 gives a quick-reference list of the CAD acronyms used in this thesis, listed in an approximately conceptual order and in alphabetical order. Figure D.1 gives a hierarchical representation of the various acronyms.

Acronym	Description
CAD	**C**ylindrical **A**lgebraic **D**ecomposition
PL-CAD	**P**rojection & **L**ifting **CAD**
RC-CAD	**R**egular **C**hains **CAD**
SICAD	**S**ign-**I**nvariant **CAD**
OICAD	**O**rder-**I**nvariant **CAD**
ECCAD	**E**quational **C**onstraint **CAD**
P-CAD	**P**artial **CAD**
TTICAD	**T**ruth **T**able **I**nvariant **CAD**
PL-TTICAD	**P**rojection & **L**ifting **T**ruth **T**able **I**nvariant **CAD**
RC-TTICAD	**R**egular **C**hains **T**ruth **T**able **I**nvariant **CAD**
L-CAD	**L**ayered sub-**CAD**
V-CAD	**V**ariety sub-**CAD**
LV-CAD	**L**ayered **V**ariety sub-**CAD**
L-TTICAD	**L**ayered **T**ruth **T**able **I**nvariant sub-**CAD**
V-TTICAD	**V**ariety **T**ruth **T**able **I**nvariant sub-**CAD**
LV-TTICAD	**L**ayered **V**ariety **T**ruth **T**able **I**nvariant sub-**CAD**

Acronym	Description
CAD	**C**ylindrical **A**lgebraic **D**ecomposition
ECCAD	**E**quational **C**onstraint **CAD**
L-CAD	**L**ayered sub-**CAD**
L-TTICAD	**L**ayered **T**ruth **T**able **I**nvariant sub-**CAD**
LV-CAD	**L**ayered **V**ariety sub-**CAD**
LV-TTICAD	**L**ayered **V**ariety **T**ruth **T**able **I**nvariant sub-**CAD**
OICAD	**O**rder-**I**nvariant **CAD**
P-CAD	**P**artial **CAD**
PL-CAD	**P**rojection & **L**ifting **CAD**
PL-TTICAD	**P**rojection & **L**ifting **T**ruth **T**able **I**nvariant **CAD**
RC-CAD	**R**egular **C**hains **CAD**
RC-TTICAD	**R**egular **C**hains **T**ruth **T**able **I**nvariant **CAD**
SICAD	**S**ign-**I**nvariant **CAD**
TTICAD	**T**ruth **T**able **I**nvariant **CAD**
V-CAD	**V**ariety sub-**CAD**
V-TTICAD	**V**ariety **T**ruth **T**able **I**nvariant sub-**CAD**

Table D.1: CAD Acronyms in conceptual and alphabetical order.

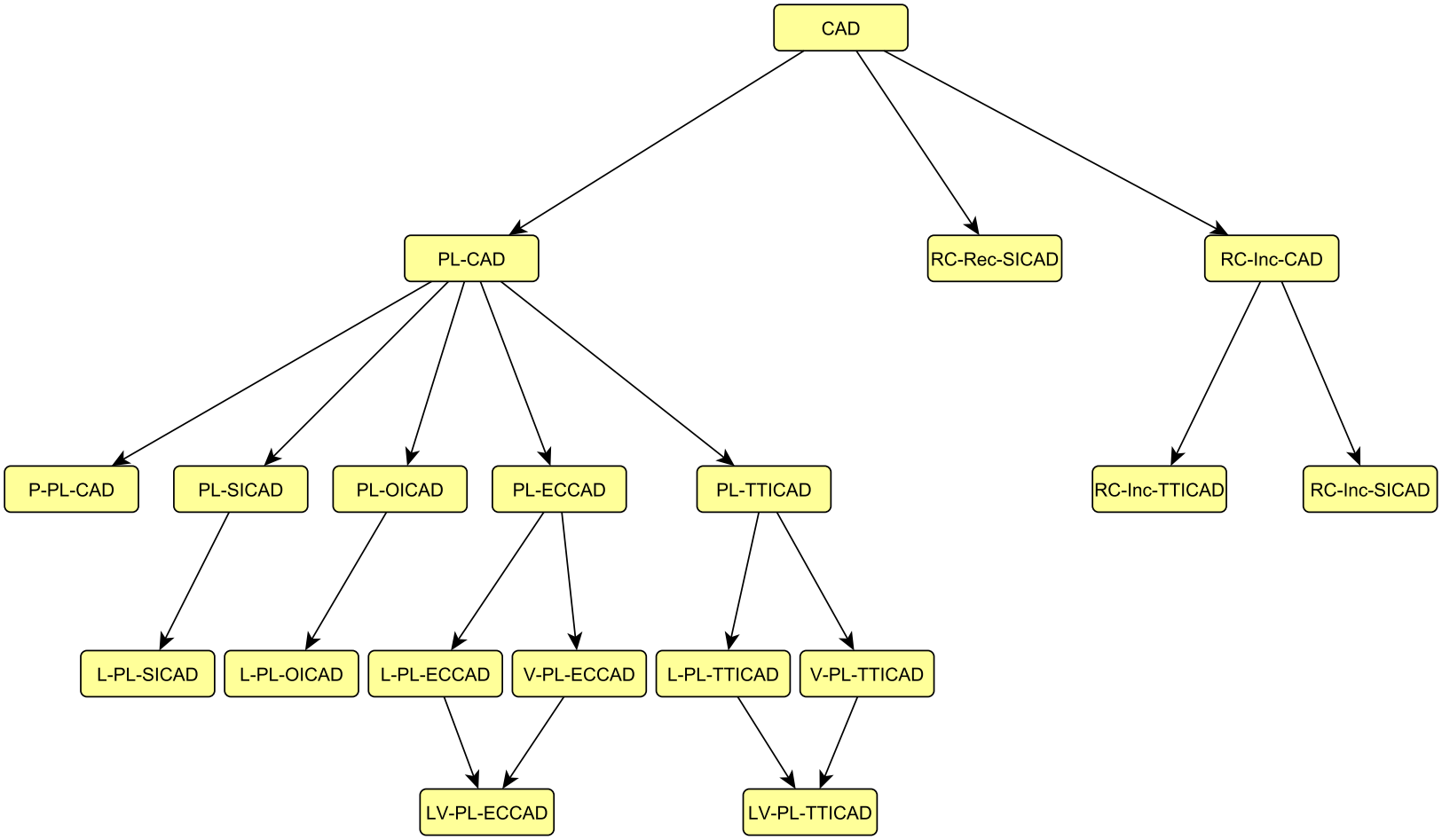


Figure D.1: A visual representation of the hierarchy of CAD acronyms.

Appendix E

Publications

A list of references to publications describing work contained in this thesis. All papers are available in their final draft form on the University of Bath Opus directory[1], in accordance to the Research Councils UK policy on open access.

E.1 Peer-Reviewed Articles

E.1.1 Published Articles

- David J. Wilson, Russell J. Bradford, and James H. Davenport. Speeding Up Cylindrical Algebraic Decomposition by Gröbner Bases. In Johan Jeuring, John A. Campbell, Jacques Carette, Gabriel Dos Reis, Petr Sojka, Makarius Wenzel, and Volker Sorge, editors, *Intelligent Computer Mathematics*, volume 7362 of *Lecture Notes in Computer Science*, pages 280–294. Springer Berlin Heidelberg, 2012 **(Refers to work in Chapter 6, Section 6.2)**.

- James H. Davenport, Russell J. Bradford, Matthew England, and David J. Wilson. Program Verification in the Presence of Complex Numbers, Functions with Branch Cuts etc. In *Proceedings of the 2012 14th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing*, SYNASC '12, pages 83–88, 2012 **(Refers to work in Chapter 6, Section 6.1)**.

- David J. Wilson, Russell J. Bradford, and James H. Davenport. A Repository for CAD Examples. *ACM Communications in Computer Algebra*, 46(3/4):67–69, January 2013 **(Refers to work in Appendix B)**.

[1]The author's Opus directory page: `http://opus.bath.ac.uk/view/person_id/6172.html`

- Russell J. Bradford, James H. Davenport, Matthew England, Scott McCallum, and David J. Wilson. Cylindrical Algebraic Decompositions for Boolean Combinations. In *Proceedings of the 38th International Symposium on Symbolic and Algebraic Computation*, ISSAC '13, pages 125–132, New York, NY, USA, 2013. ACM **(Refers to work in Chapter 3)**.

- David J. Wilson, James H. Davenport, Matthew England, and Russell J. Bradford. A "Piano Movers" Problem Reformulated. In *Proceedings of the 15th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing*, SYNASC '13, pages 53–60, Sept 2013 **(Refers to work in Chapter 6, Section 6.3)**.

- Russell J. Bradford, James H. Davenport, Matthew England, and David J. Wilson. Optimising Problem Formulation for Cylindrical Algebraic Decomposition. In Jacques Carette, David Aspinall, Christoph Lange, Petr Sojka, and Wolfgang Windsteiger, editors, *Intelligent Computer Mathematics*, volume 7961 of *Lecture Notes in Computer Science*, pages 19–34. Springer Berlin Heidelberg, 2013 **(Refers to work in Chapters 3 and 5)**.

- Matthew England, Russell J. Bradford, James H. Davenport, and David J. Wilson. Understanding Branch Cuts of Expressions. In Jacques Carette, David Aspinall, Christoph Lange, Petr Sojka, and Wolfgang Windsteiger, editors, *Intelligent Computer Mathematics*, volume 7961 of *Lecture Notes in Computer Science*, pages 136–151. Springer Berlin Heidelberg, 2013 **(Refers to work in Chapter 3, Section 3.9)**.

- Matthew England, Edgardo Cheb-Terrab, Russell J. Bradford, James H. Davenport, and David J. Wilson. Branch Cuts in Maple 17. *ACM Communications in Computer Algebra*, 48(1/2):24–27, March 2014 **(Refers to work in Chapter 3, Section 3.9)**.

- David J. Wilson, Russell J. Bradford, James H. Davenport, and Matthew England. Cylindrical Algebraic Sub-Decompositions. *Mathematics in Computer Science*, 8(2):263–288, 2014 **(Refers to work in Chapter 4)**.

- Matthew England, Russell J. Bradford, Changbo Chen, James H. Davenport, MarcMoreno Maza, and David J. Wilson. Problem Formulation for Truth-Table Invariant Cylindrical Algebraic Decomposition by Incremental Triangular Decomposition. In Stephen M. Watt, James H. Davenport, Alan P. Sexton, Petr Sojka, and

Josef Urban, editors, *Intelligent Computer Mathematics*, volume 8543 of *Lecture Notes in Computer Science*, pages 45–60. Springer International Publishing, 2014 **(Refers to work in Chapters 3 and 5)**.

- Zongyan Huang, Matthew England, David J. Wilson, James H. Davenport, Lawrence C. Paulson, and James Bridge. Applying Machine Learning to the Problem of Choosing a Heuristic to Select the Variable Ordering for Cylindrical Algebraic Decomposition. In Stephen M. Watt, James H. Davenport, Alan P. Sexton, Petr Sojka, and Josef Urban, editors, *Intelligent Computer Mathematics*, volume 8543 of *Lecture Notes in Computer Science*, pages 92–107. Springer International Publishing, 2014 **(Refers to work in Chapter 5, Section 5.3)**.

E.1.2 Accepted for publication/presentation

- Zongyan Huang, Matthew England, David J. Wilson, James H. Davenport, and Lawrence C. Paulson. A comparison of three heuristics to choose the variable ordering for cylindrical algebraic decomposition. *ACM Communications in Computer Algebra*, 2014 **(Accepted to *ISSAC 2014* poster session to be published in *Communications in Computer Algebra*; refers to work in Chapter 5, Section 5.3.5)**.

- Matthew England, David J. Wilson, Russell J. Bradford, and James H. Davenport. Using the Regular Chains Library to build cylindrical algebraic decompositions by projecting and lifting. In *Proceedings of the 2014 International Congress on Mathematical Software*, 2014 **(Accepted to *ICMS 2014*; refers to work in Appendix C)**.

- Matthew England, Russell J. Bradford, James H. Davenport, and David J. Wilson. Choosing a variable ordering for truth-table invariant cylindrical algebraic decomposition by incremental triangular decomposition. In *Proceedings of the 2014 International Congress on Mathematical Software*, 2014 **(Accepted to *ICMS 2014*; refers to work in Chapters 3 and 5)**.

- Russell J. Bradford, Changbo Chen, James H. Davenport, Matthew England, Marc Moreno Maza, and David J. Wilson. Truth Table Invariant Cylindrical Algebraic Decomposition by Regular Chains. *CoRR*, abs/1401.6310, 2014 **(Accepted to *CASC 2014*; refers to work in Chapter 3)**.

- David J. Wilson, Matthew England, Russell J. Bradford, and James H. Davenport. Using the distribution of cells by dimension in a cylindrical algebraic decomposition. *SYNASC 2014*, 2014 **(Accepted to *SYNASC 2014*; refers to work in Section 5.4)**.

E.1.3 Submitted for consideration

- Russell J. Bradford, James H. Davenport, Matthew England, Scott McCallum, and David J. Wilson. Truth Table Invariant Cylindrical Algebraic Decomposition. *CoRR*, abs/1401.0645, 2014 **(Submitted to *Journal of Symbolic Computation*; refers to work in Chapter 3)**.

E.2 Non-Peer-Reviewed Articles

E.2.1 University of Bath Technical Reports

- David J. Wilson. *Real Geometry and Connectedness via Triangular Description: CAD Example Bank*. Opus: University of Bath Online Publication Store, 2012 **(Refers to work in Appendix B)**.

- David J. Wilson and Matthew England. Layered Cylindrical Algebraic Decomposition. Technical report, Bath, August 2013 **(Refers to work in Chapter 4)**.

- David J. Wilson, Russell J. Bradford, James H. Davenport, and Matthew England. The Piano Mover's Problem Reformulated. Technical report, Bath, June 2013 **(Refers to work in Chapter 6)**.

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[BCD+14] Russell J. Bradford, Changbo Chen, James H. Davenport, Matthew England, Marc Moreno Maza, and David J. Wilson. Truth Table Invariant Cylindrical Algebraic Decomposition by Regular Chains. *CoRR*, abs/1401.6310, 2014.

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[BDE+14] Russell J. Bradford, James H. Davenport, Matthew England, Scott McCallum, and David J. Wilson. Truth Table Invariant Cylindrical Algebraic Decomposition. *CoRR*, abs/1401.0645, 2014.

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Index